Volume 68B
Number 4
Oct.–Dec. 1964

Mathematics and Mathematical Physics

U.S. DEPARTMENT OF COMMERCE

SECTION B

JOURNAL OF RESEARCH

NATIONAL BUREAU OF STANDARDS

Journal of Research

of the

National Bureau of Standards

B. Mathematics and Mathematical Physics

OCT.–DEC. • 1964

VOLUME • 68B

NUMBER • 4

Editor: Chester H. Page

Associate Editors: William H. Pell, John J. Sopka

Publication dates: Mar. 10, June 10, Sept. 10, Dec. 10, 1964

JOURNAL OF RESEARCH

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JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 68B, No. 4, October–December 1964

Hydrodynamic Fluctuations and Stokes' Law Friction

Robert Zwanzig

(September 3, 1964)

The frictional force on a Brownian motion particle can be expressed by means of the time-correlation of the fluctuating force on the particle. We show that this method, applied to a spherical particle in a viscous incompressible fluid, leads to Stokes' Law. The calculation is based on the theory of hydrodynamic fluctuations due to Landau and Lifshitz, and on a hydrodynamic theorem due to Faxen.

The subject of this article is the connection between two different methods for calculating the frictional force on a Brownian motion particle. One method is based on the statistical mechanical theory of irreversible processes, and involves evaluation of a certain time-correlation formula. The other method is based on macroscopic hydrodynamics, and requires solution of the Navier-Stokes equation.

For simplicity we restrict the discussion to the special case of a spherical particle of radius a moving slowly through a viscous incompressible fluid. The viscosity coefficient is η.

In the hydrodynamic theory, the frictional force $\mathbf{F}$ on a sphere moving with constant velocity $\mathbf{v}$ is given by Stokes' law,

$$\mathbf{F} = -\zeta \mathbf{v}, \tag{1}$$

$$\zeta = 6\pi\eta a. \tag{2}$$

In the molecular theory, eq (1) is unchanged; but the friction constant is now given by a time-correlation formula. This formula was obtained first by Kirkwood [1].[1] A more precise and general treatment has been given by Lebowitz and Rubin [2].

The time-correlation formula for ζ is

$$\zeta = \frac{1}{3k_B T} \lim_{\epsilon \to 0} \int_0^\infty dt\, e^{-\epsilon t} \left\langle \mathbf{F}(0) \cdot \mathbf{F}(t) \right\rangle. \tag{3}$$

In this expression, $\mathbf{F}(t)$ is the total force exerted on the sphere at time t by the molecules in the surrounding fluid. The time dependence of $\mathbf{F}(t)$ is determined by solution of the molecular equations of motion, subject only to the condition that the spherical particle is held fixed in position. The angular bracket $\langle\ \rangle$ denotes an average over a thermal equilibrium ensemble at temperature T. Boltzmann's constant is k_B.

[1] Figures in brackets indicate the literature references at the end of this paper.

The time-correlation formula (3) is known to be much more general than Stokes' formula (2). For example, Green [3] and Mazo [4] have shown that it gives the correct expression for the friction constant in a Rayleigh gas, where the molecular mean free path is much greater than the radius of the sphere. Stokes' formula, having been derived only in the hydrodynamic limit (mean free path much smaller than the radius of the sphere), is not valid for a Rayleigh gas.

In this article we show the equivalence of (2) and (3) under conditions where the hydrodynamic result is valid. Our discussion is based on the statistical theory of hydrodynamic fluctuations, as set forth by Landau and Lifshitz [5].

In the Landau-Lifshitz theory, as applied to a viscous incompressible fluid at low Reynolds number, the equations of motion are the conservation law

$$\nabla \cdot \mathbf{v} = 0, \tag{4}$$

and the generalized Navier-Stokes equation

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\nabla p + \eta \nabla^2 \mathbf{v} + \nabla \cdot \mathbf{S} \tag{5}$$

with the convective inertial terms omitted because of the low Reynolds-number application. The pressure is p; the fluid density is ρ; and $\mathbf{S}$ is the fluctuation of the stress tensor away from the value it takes on when the fluid is in *local* thermodynamic equilibrium (i.e., the deviation from the usual Navier-Stokes stress tensor).

In the language of Brownian motion theory, eq (5) may be regarded as a Langevin equation. The divergence of $\mathbf{S}$ represents the fluctuating force acting on the fluid. This force is not specified exactly, but only in a statistical way. In particular, its mean value vanishes, and its second moment is given by

$$\langle \mathbf{S}_{ik}(\mathbf{r}_1, t_1) \mathbf{S}_{lm}(\mathbf{r}_2, t_2) \rangle = 2k_B T \eta \Big[\delta_{il}\delta_{km} + \delta_{im}\delta_{kl} - \frac{2}{3}\delta_{ik}\delta_{lm} \Big] \times \delta(\mathbf{r}_1 - \mathbf{r}_2) \times \delta(t_1 - t_2). \tag{6}$$

(We have left out certain terms containing the coefficient of volume viscosity, since we are concerned with only incompressible fluids.)

Note that the correlation is taken to be local in space and time, as indicated by the delta functions in eq (6). This is an approximation which must fail for molecular times and distances; but because we are interested in only macroscopic times and distances, the approximation is good enough.

Because eq (5) is a Langevin equation, the probability distribution of velocities is given by a certain Fokker-Planck equation; this connection is quite familiar in the theory of Brownian motion. The appropriate Fokker-Planck equation is in fact the basic kinetic equation of Green's theory of irreversible processes in fluids [6].

As in the usual hydrodynamic derivation of Stokes' law, we assume all macroscopic processes to be so slow that the time derivative in eq (5) can be neglected.

Fluctuations in the local stress tensor give rise to fluctuations in the local pressure and velocity fields, and consequently to fluctuations in the total force on a sphere. When the fluid is at equilibrium, the mean velocity vanishes and the mean pressure is spatially uniform; so the mean force on the sphere vanishes. Thus we need to take account of only deviations from the mean behavior of the fluid.

To find the actual velocity and pressure fields associated with the fluctuating stress tensor, it appears at first that we must solve the hydrodynamic eqs (4) and (5) subject to the boundary condition $\mathbf{v}(\mathbf{r}, t)=0$ on the surface of the sphere. This calculation is a moderately difficult one. Fortunately, however, one can find the total force on the sphere using only the "unperturbed" velocity field that prevails in the absence of the sphere, by means of a remarkable theorem due to Faxen [7]. According to this theorem, the force $\mathbf{F}(t)$ on a sphere fixed at the origin, caused by an unperturbed velocity field $\mathbf{v}(\mathbf{r}, t)$, is

$$\mathbf{F}(t)=6\pi\eta a\cdot\frac{1}{4\pi}\oint d\Omega\mathbf{v}(\mathbf{r}, t). \tag{7}$$

This equation evidently resembles Stokes' law, except that the velocity of the sphere has been replaced by the negative of the unperturbed velocity of the fluid, *averaged over the surface of the sphere.* ($\oint d\Omega/4\pi$ denotes an average over all angles.)

It is easy to see that Stokes' law is a special case of Faxen's theorem.

The only conditions needed for the validity of Faxen's theorem are the ones we have already imposed: incompressibility, and omission of the time derivative in the Navier-Stokes equation.

To apply Faxen's theorem, we need the fluctuating velocity field for a medium that is at equilibrium, spatially uniform (no spherical particle present!), and infinite in extent. The calculation of this velocity field is performed easily by means of Fourier transforms.

Thus, we write any function $f(\mathbf{r})$ of position $\mathbf{r}$ as an integral,

$$f(\mathbf{r})=\int d^3k f_k \exp i\mathbf{k}\cdot\mathbf{r}. \tag{8}$$

In particular, the Fourier transform of eq (6) is

$$\langle S_{ik}(\mathbf{k}_1, t_1)S_{lm}(\mathbf{k}_2, t_2)\rangle = \frac{2k_BT\eta}{(2\pi)^3}\left[\delta_{il}\delta_{km}+\delta_{im}\delta_{kl}-\frac{2}{3}\delta_{ik}\delta_{lm}\right] \times\delta(\mathbf{k}_1+\mathbf{k}_2)\delta(t_1-t_2). \tag{9}$$

The conservation law (4) becomes

$$\mathbf{k}\cdot\mathbf{v}_\mathbf{k}=0,$$

and the Navier-Stokes eq (5) becomes (on omission of the time-derivative)

$$0=-i\mathbf{k}p_\mathbf{k}-\eta k^2\mathbf{v}_\mathbf{k}+i\mathbf{k}\cdot\mathbf{S}(\mathbf{k}). \tag{11}$$

The pressure is found by multiplying eq (11) by $\mathbf{k}$,

$$p_k=\mathbf{kk}:\mathbf{S}(\mathbf{k})/\mathbf{k}^2. \tag{12}$$

Then the velocity is

$$\mathbf{v}_\mathbf{k}=\frac{1}{\eta k^2}\{i\mathbf{k}\cdot\mathbf{S}(\mathbf{k})-i\mathbf{kkk}:\mathbf{S}(\mathbf{k})/k^2\}. \tag{13}$$

The velocity correlation is found easily from eqs (13) and (9),

$$\langle\mathbf{v}(\mathbf{k}_1, t_1)\mathbf{v}(\mathbf{k}_2, t_2)\rangle=\frac{4k_BT}{\eta}\frac{1}{(2\pi)^3}\frac{1}{k_1^2}\delta(\mathbf{k}_1+\mathbf{k}_2)\delta(t_1-t_2). \tag{14}$$

The mean force $\langle\mathbf{F}(t)\rangle$ vanishes, because the mean fluctuating stress tensor vanishes. But the correlation in the fluctuating force does not vanish. This is precisely the quantity we need for the present calculation.

Let us rewrite eq (7) using Fourier components,

$$\mathbf{F}(t)=6\pi\eta a\int d^3k\frac{\sin ka}{ka}\mathbf{v}(\mathbf{k}, t). \tag{15}$$

On using eq (14) we obtain

$$\langle\mathbf{F}(0)\cdot\mathbf{F}(t)\rangle=(6\pi\eta a)^2\int d^3k_1\int d^3k_2 \times\frac{\sin k_1a}{k_1a}\frac{\sin k_2a}{k_2a}\langle\mathbf{v}(\mathbf{k}_1, 0)\cdot\mathbf{v}(\mathbf{k}_2, t)\rangle = 18\frac{k_BT\eta a^2}{\pi}\int d^3k\frac{1}{k^2}\left(\frac{\sin ka}{ka}\right)^2\delta(t). \tag{16}$$

The remaining integral is elementary, and the result is

$$\langle\mathbf{F}(0)\cdot\mathbf{F}(t)\rangle=36\pi k_BT\eta a\delta(t). \tag{17}$$

To complete the derivation, we need only to put (17) into (3). Because the time integration runs from $t=0$ to $t=\infty$, and not from $t=-\infty$ to $t=\infty$, we pick up only half of the delta function. This gives

$$\zeta=6\pi\eta a, \tag{18}$$

in complete agreement with Stokes' law.

It should be noted that we have not actually *derived* Stokes' law from the time-correlation formula. In fact, Stokes' law (or rather, Faxen's generalization) played an essential role in the preceding discussion. Nevertheless, the argument is not circular; the generalized Navier-Stokes-Langevin equation, together with eq (6) for the correlation in the fluctuating stress tensor, cannot be obtained from purely hydrodynamic arguments. Similarly, the time-correlation formula for the friction constant cannot be obtained from hydrodynamics. A statistical theory is needed.

If one wished to derive Stokes' law directly from molecular theory, the most natural procedure would be first to derive the fundamental hydrodynamic laws from molecular theory. But having obtained the hydrodynamic laws, one might as well use them to get Stokes' law. In other words, the time-correlation formula is hardly necessary. All we have done in this article is to show how the time-correlation formula gives the same results as the hydrodynamic theory under conditions where the hydrodynamic theory is already available.

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(Paper 68B4–126)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 68B, No. 4, October–December 1964

Equivalence of Certain Inequalities Complementing Those of Cauchy-Schwarz and Hölder

J. B. Diaz,[1] A. J. Goldman, and F. T. Metcalf [1]

(August 26, 1964)

An inequality due to the first and third authors, which complements the Cauchy-Schwarz Inequality, is shown equivalent to a result of Rennie. A more general inequality due to the first and third authors, which complements that of Hölder, is proven equivalent to a previously published generalization of Rennie's Inequality.

Although the inequalities treated below have discrete analogs [2; 4] [2] as well as Hilbert space operator analogs [6], we shall present only the integral versions. The symbol I will denote integration over a fixed totally finite measure space, the existence and finiteness of the various definite integrals involved being assumed throughout. M and m stand for real numbers with $M > m$.

In [2; 5], Diaz and Metcalf give the following result for real-valued functions f and g with the former nonvanishing: *If*

$$m \leq g/f \leq M \tag{1}$$

almost everywhere, then

$$I(g^2) + mMI(f^2) \leq (M+m)I(fg) \tag{2}$$

with equality if and only if

$$(M - g/f)(g/f - m) = 0 \tag{3}$$

almost everywhere. Since (2) gives a lower bound for the "inner product" $I(fg)$ in terms of the squares of the "norms" $\{I(f^2)\}^{1/2}$ and $\{I(g^2)\}^{1/2}$, it can be regarded as a complement to the Cauchy-Schwarz Inequality

$$I(fg) \leq \{I(f^2)\}^{1/2}\{I(g^2)\}^{1/2}$$

which yields an *upper* bound for the inner product in terms of the norms.

In [11], Rennie shows for a real-valued function F that *if*

$$0 < m \leq F \leq M \tag{4}$$

almost everywhere, then

$$I(F) + MmI(F^{-1}) \leq (M+m)I(1) \tag{5}$$

with equality if and only if

$$(M - F)(F - m) = 0 \tag{6}$$

almost everywhere. Our first aim in this note is to exhibit the equivalence between Rennie's Inequality and the one given in the last paragraph.

First, suppose it "given" that (1) implies (2). If F obeys (4), we can set

$$g = F^{1/2}, f = F^{-1/2}$$

in (2) to obtain (5), and can observe that (3) applies if and only if (6) does.

Second, suppose it "given" that (4) implies (5). Let f and g obey (1), and initially assume $m > 0$. Then $fg > 0$ almost everywhere, so that from the original measure μ we can obtain a new measure μ' given by

$$\mu'(S) = I(fgC_S)$$

where C_S is the characteristic function of S. Let I' denote integration over the entire space with respect to μ'. Then f and g obey (1) almost everywhere (μ') as well as (μ), so that (4) with $F = g/f$ yields from (5)

$$I'(g/f) + MmI'(f/g) \leq (M+m)I'(1)$$

which is equivalent to the desired result (2). Moreover equality holds in (2) if and only if it holds almost everywhere (μ') in (6), hence iff it holds almost everywhere (μ') in (3), thus iff it holds almost everywhere (μ) in (3).

If the hypothesis $m > 0$ is dropped, we need only choose a real number c so large that $m + c > 0$, and replace (1) with its consequence

$$0 < m + c \leq (g + cf)/f \leq M + c.$$

[1] Institute for Fluid Dynamics and Applied Mathematics, University of Maryland; research supported in part by the Air Force Office of Scientific Research—Grant AFOSR 400-64.

[2] Figures in brackets indicate the literature references at the end of this paper.

By the case just treated we have

$$I((g+cf)^2)+(m+c)(M+c)I(f^2) \leq (M+c+m+c)I(f(g+cf))$$

with equality if and only if (3) holds almost everywhere. The terms in c on both sides of this last inequality (after expansion) are identical, and can be subtracted off to obtain the desired result (2). This completes the proof of equivalence.

Now let p and q be real numbers which are "Hölder-conjugate," i.e.,

$$p>0, q>0, p^{-1}+q^{-1}=1. \tag{7}$$

In [3], Diaz and Metcalf announced the discrete analog of the following result for a positive-valued function f and a nonnegative-valued function g: *If*

$$0 \leq m^p \leq g^q/f^p \leq M^p \tag{8}$$

almost everywhere, then

$$(M-m)^{-1}(M^{p-1}-m^{p-1})I(g^q) + (Mm)^{p-1}I(f^p) \leq (M-m)^{-1}(M^p-m^p)I(fg) \tag{9}$$

with equality if and only if

$$(M^p-g^q/f^p)(g^q/f^p-m)=0 \tag{10}$$

almost everywhere. Since (9) gives a lower bound for the "bilinear product" $I(fg)$ in terms of the "conjugate norms" $\{I(f^p)\}^{1/p}$ and $\{I(g^q)\}^{1/q}$, it can be regarded as a complement to the Hölder Inequality

$$I(fg) \leq \{I(f^p)\}^{1/q}\{I(g^q)\}^{1/q}$$

which yields a corresponding *upper* bound. Note that (1) and (2) constitute the special case $p=q=2$ of this result.

We shall find it convenient to "normalize" this result by a technique which fails in case $m=0$, and therefore note in advance that an elementary proof is available in case $m=0$: From (8) we obtain $0 \leq g^q \leq M^p f^p$, so that

$$g^q = g^{q-1}\cdot g = (g^q)^{(q-1)/q}\cdot g = (g^q)^{1/p}\cdot g \leq Mfg$$

almost everywhere, implying

$$I(g^q) \leq MI(fg)$$

which is equivalent to (9) with $m=0$; (10) also comes out right.

Assuming now that $m>0$ in (8), we "normalize" by replacing m by 1, M by the constant $Q=M/m>1$, and g by the function $h=g/m$. The equivalent normalized version of the result [3] then reads as follows: *If* $p>1$, *and if the positive-valued functions* f *and* h *satisfy*

$$1 \leq h/f \leq Q \tag{11}$$

almost everywhere, then

$$(Q^p-Q^{p-1})I(f^p) \leq (Q^p-1)I(fh^{p-1})-(Q^{p-1}-1)I(h^p) \tag{12}$$

with equality if and only if

$$(Q-h/f)(h/f-1)=0 \tag{13}$$

almost everywhere. Here $p>1$ is the necessary and sufficient condition for p to be related to some q as in (7).

In [8], Goldman proved and presented as a normalized generalization of Rennie's Inequality, the following result, which turns out to have been anticipated by Rennie himself (see example 1 of [12]) and also to appear in recent work of A. W. Marshall and I. Olkin [10]: Let s and r be real numbers satisfying

$$s>r, sr\neq 0. \tag{14}$$

If the function F *satisfies*

$$1 \leq F \leq Q \tag{15}$$

almost everywhere, then

$$(Q^s-Q^r)I(1) \leq (Q^s-1)I(F^r)-(Q^r-1)I(F^s) \text{ if } sr>0, \tag{16a}$$

$$(Q^s-Q^r)I(1) \geq (Q^s-1)I(F^r)-(Q^r-1)I(F^s) \text{ if } sr<0, \tag{16b}$$

with equality if and only if

$$(Q-F)(F-1)=0 \tag{17}$$

almost everywhere. (The additional normalization $I(1)=1$ was assumed in [8].) Our second aim is to exhibit the equivalence between this result and the one given in the last paragraph.

First assume it "given" that (11) implies (12). Let F obey (15), and suppose initially that $s>r>0$. Introduce the numbers

$$p=s/(s-r)>1, \overline{Q}=Q^{s-r}$$

so that

$$\overline{Q}^p=Q^s, \overline{Q}^{p-1}=Q^r,$$

and (15) implies that $1 \leq F^{s-r} \leq \overline{Q}$ almost everywhere. Application of (12) with $\overline{Q}$ replacing Q, $h=F^{s-r}$, and $f=1$, yields (16a) as desired. The argument shows that equality holds in (16a) if and only if the analog

$$(\overline{Q}-F^{s-r})(F^{s-r}-1)=0$$

of (13) holds almost everywhere, which is equivalent to (17).

Next suppose $0>s>r$, and set

$$s'=-r, r'=-s, \overline{F}=QF^{-1}$$

so that

$$s' > r' > 0, 1 \leq \overline{F} \leq Q.$$

By the case of (16a) already proved,

$$(Q^{-r} - Q^{-s})I(1) \leq (Q^{-r} - 1)I(\overline{F}^{-s}) - (Q^{-s} - 1)I(\overline{F}^{-r}), \quad (18)$$

i.e.,

$$(Q^{-r} - Q^{-s})I(1) \leq (Q^{-r} - Q^{-r-s})I(F^r) - (Q^{-s} - Q^{-r-s})I(F^s)$$

which is equivalent to (16a) after multiplication by Q^{s+r}. Furthermore, equality holds if and only if

$$(Q - \overline{F})(\overline{F} - 1) = 0$$

almost everywhere, which is seen to be equivalent to (17) after multiplying the first factor by $FQ^{-1} > 0$ and the second by $F > 0$.

Finally suppose $s > 0 > r$, and set

$$s' = s - r, r' = -r,$$

so that $s' > r' > 0$. Introduce a new measure μ' (and corresponding integration I') related to the original measure μ by

$$\mu'(S) = Q^r I(F^r C_S).$$

Then (15) holds almost everywhere (μ') since it holds almost everywhere (μ); applying the already-proven (16a) with s' and r' replacing s and r yields

$$(Q^{s-r} - Q^{-r})I'(1) \leq (Q^{s-r} - 1)I'(F^{-r}) - (Q^{-r} - 1)I'(F^{s-r}),$$

or equivalently

$$(Q^{s-r} - 1)I'(F^{-r}) \geq (Q^{s-r} - Q^{-r})I'(1) - (1 - Q^{-r})I'(F^{s-r}),$$

which is in turn equivalent to the desired result (16b), the condition for equality also working out correctly.

Second, assume it "given" that (15) implies (16). Suppose that h and f satisfy (11) and that $p > 1$. Introduce a new measure μ' (and corresponding integration I') related to the original measure μ by

$$\mu'(S) = I(f^p C_S).$$

Taking $F = h/f$ in (15) with $s = p$ and $r = p - 1$ leads *via* (16a) to

$$(Q^p - Q^{p-1})I'(1) \leq (Q^{p-1})I'(h^{p-1}/f^{p-1}) - (Q^{p-1} - 1)I'(h^p/f^p)$$

which is equivalent to the desired result (12), the condition for equality also working out correctly. This completes the equivalence proof.

Two final remarks are in order. *First*, a number of known inequalities can be obtained by weakening the ones given here or their discrete or operator analogs, e.g., by applying to one side the relation between arithmetic and geometric means. This particular process when applied to (16) yields the upper bounds for ratios of weighted means obtained by Cargo and Shisha [1], as was noted in [8] and [12]; when applied to (9) it yields an inequality due to Gheorghiu [7], which our results therefore show to be equivalent to the Cargo-Shisha bounds. The specifics for other corollaries are given in the papers cited. *Second*, the justification for the measure-theoretic maneuvers employed (the transitions between μ and I, and μ' and I') is supplied by appeal to Halmos [9; p. 134].

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(Paper 68B4–127)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 68B, No. 4, October–December 1964

Weak Generalized Inverses and Minimum Variance Linear Unbiased Estimation

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(August 25, 1964)

This paper presents a unified account of the theory of least squares and its adaptations to statistical models more complicated than the classical one. First comes a development of the properties of weak generalized matrix inverses, a useful variant of the more familiar pseudo-inverse. These properties are employed in a proof of the usual Gauss theorem, and in analyzing the case in which known linear restraints are obeyed by the parameters. Another situation treated is that of a singular variance-covariance matrix for the observations. Applications include the case of equi-correlated variables (including estimation despite ignorance of the correlation), linear "restraints" subject to random error, and stepwise linear estimation.

1. Introduction and Summary

The aim of this paper is to present a unified account of the theory of least squares, and in particular to describe the necessary modifications when the customary statistical model is complicated in certain ways required for greater realism. The paper contains (probably) new results, (probably) new proofs of known results, and an (almost certainly) new overall treatment of the subject. Our hesitancy to make stronger claims arises because many of the theorems associated with least squares are part of the "folk-lore" of the field, and because the relevant literature is growing rapidly and much of it is "disguised" in the context of other branches of mathematics or science. The most closely related paper of which we are aware of is that of Rao [1962]; our work was done independently of his. (The relevance of the very recent paper of Chipman and Rao [1964], which contains other references of interest, is detailed at the end of section 5.2.) Valuable summaries of various aspects of the theory of least squares can be found in Deming [1943], Plackett [1949, 1960], Rao [1946], and Scheffe [1959].

The foundation of least-squares estimation theory is the well-known Gauss[2] theorem which can be proved in a number of ways, e.g., by linear vector space techniques as in Scheffe (*op. cit*) or by the method of Lagrange multipliers as in Plackett [1960]. We shall present a proof suggested by the properties of generalized inverses of matrices, an idea motivated quite naturally by the possible singularity of the coefficient matrix in the usual normal equations. It will be shown that any one of a wider class of matrices, which we call *weak generalized inverses*, can serve equally well. The properties of weak generalized inverses appear interesting in their own right; they are developed in section 2, are applied to the derivation of the Gauss theorem in section 3, and are involved implicitly or explicitly throughout the rest of the paper as well.

One complication of the customary statistical model which often arises in practice is the imposition of known linear restraints on the parameters. In section 4 the Gauss theorem is extended to this case. For a careful analysis it is important to distinguish clearly between artificial constraints (imposed to obtain unique solutions) and "real" ones, and among the latter class to exploit the distinction between those constrained functions which were estimable before the restraints were imposed and those which are estimable only by virtue of the restraints.

Another frequent complication, the possibility of a singular variance-covariance matrix for the observations, is discussed in section 5. It is shown how this deviation from the "standard model" can be replaced by the adjunction of linear restraints, and *vice versa*. Models involving *both* kinds of complications are treated. Applications of the general theory are made to the case of equicorrelated variables (including the possibility of estimation in some cases despite ignorance of the correlation), and to the case of linear "restraints" subject to random error. The topic of *stepwise linear estimation*, which has aroused considerable interest recently, is examined in section 5.5(cf. Freund, Vail, and Clunies-Ross [1961], Goldberger and Jockems [1961]).

The style of the paper represents a compromise between (1) the desire to have it serve as a useful

*Part of this author's work was supported by the Mathematics Research Center, U.S. Army, Madison, Wis. under Contract DA–11–022–Ord–2059. This is a revision and extension of Mathematics Research Center Technical Report 314, May 1962.

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[2] The literature refers to Gauss' fundamental work as the Markov or the Gauss-Markov theorem. Since Markov's contribution consisted essentially of bringing attention to Gauss' work, it does not appear necessary to hyphenate the theorem with the name of Markov.

statistical reference as well as a vehicle of research communication, and (2) the need to avoid a length and prolixity which surely would induce "battle fatigue" in readers and authors alike. On the one hand, additional information and "sidelights" appear throughout as corollaries and informal remarks. Also, the more familiar matrix techniques have been used in preference to vector space concepts, at the cost of some awkwardness at points where the "linear geometry" approach is the really natural one. Proofs have been written out in fairly full detail (except for matrix-algebraic steps). It is hoped that these policies make the paper more valuable and accessible to a wider range of readers. On the other hand, it has been necessary to presuppose a rather mature grasp of matrix theory and manipulations. A serious expository gap (which we hope some colleague will fill) is the omission of any discussion of computational methods for the calculations required in utilizing the theory, and also the absence of concrete and non-trivial numerical examples. Inclusion of such material, though desirable for completeness, would have interrupted the logical pattern of the theoretical development.

It is a pleasure to acknowledge the many fruitful, often heated, but always stimulating discussions with J. M. Cameron (NBS Statistical Engineering Laboratory) which have continued over many years. Without his constant interest, this paper would never have been written. Colleagues at the Mathematics Research Center, whose helpful comments have influenced the present version of the material, include H. Reinhardt and J. C. Boot. We also acknowledge with thanks a constructive reading of our paper by T. N. E. Greville.

2. Weak Generalized Inverses

In this section we define weak generalized inverses and develop some of their properties. Let X be a $p \times n$ matrix. As a special case of what follows, we shall show that there exists an $n \times p$ matrix X^+ with the properties [3]

$$\begin{aligned} &\text{(a)} \quad XX^+X = X \\ &\text{(b)} \quad X^+XX^+ = X^+ \\ &\text{(c)} \quad (X^+X)' = X^+X \\ &\text{(d)} \quad (XX^+)' = XX^+. \end{aligned} \tag{2.1}$$

The matrix X^+ is unique (this will not be proved in the present paper) and is called the generalized inverse of X. Further details on this topic can be found in the excellent review paper by Greville [1959]. Sometimes X^+ is called a pseudo-inverse or a Moore-Penrose inverse, the latter association referring to Moore [1935] who originally discovered its properties, and to Penrose [1953] who later rediscovered and developed them further.

[3] A superscript prime will always denote (vector or matrix) transposition; the original definitions involved the complex-conjugate transpose, but we deal only with real matrices.

Our approach to this material is based on the following lemmas whose proofs (although simple) are given for completeness.

LEMMA 1. *Let* A *be a* p×p *symmetric matrix of rank* q (q < p), *and* K *a* p×r *matrix of rank* r = p − q. *Then there exists a* p×r *matrix* H *with the properties*

$$\begin{aligned} &\text{(a)} \quad H'A = 0 \\ &\text{(b)} \quad \det(H'K) \neq 0 \end{aligned} \tag{2.2}$$

if and only if the square symmetric matrix

$$M = \begin{bmatrix} A & K \\ K' & 0 \end{bmatrix}$$

is nonsingular. In this case any H *of rank* r *obeying* (2.2a) *can be used as the* H *in* (2.2b). *Furthermore,* M^{-1} *has the form*

$$M^{-1} = \begin{bmatrix} C & \vdots & H(K'H)^{-1} \\ \cdots & \cdots & \cdots \\ (H'K)^{-1}H' & \vdots & 0 \end{bmatrix}.$$

PROOF. First assume M nonsingular, and let

$$M^{-1} = \begin{bmatrix} C & C_1 \\ C_1' & C_2 \end{bmatrix}$$

where C is symmetric and $p \times p$, C_2 is symmetric and $r \times r$, and C_1 is $p \times r$. The multiplication [4] $MM^{-1} = I$ implies

$$AC + KC_1' = I.$$

Now choose any $p \times r$ matrix H of rank r obeying (2.2a). Such matrices certainly exist. Premultiply the last equation by H' to obtain $H'KC_1' = H'$; since H' is of rank r, $H'K$ must have rank $\geq r$ (and thus exactly r since K has rank r), so that (2.2b) holds. To prove the converse, let H be any $p \times r$ matrix obeying (2.2). Then by (2.2b) H must have rank $r = p - q$, and from this and (2.2a) it follows that any $p \times p$ matrix B with $H'B = 0$ has the form $B = AD$ for some $p \times p$ matrix D. Now specialize to $B = I - K(H'K)^{-1}H'$ and use the resulting matrix D to define [5]

$$C = [I - H(K'H)^{-1}K']D.$$

If this matrix, together with $C_1 = H(K'H)^{-1}$ and $C_2 = 0$, is substituted in the M^{-1} formula given above, then it is easily verified that $MM^{-1} = I$ so that M is nonsingular and the proof is complete.

[4] The symbol I will always denote an identity matrix of appropriate dimension.

[5] We remark that the matrix C can be written explicitly as $C = [I - H(K'H)^{-1}K'][A + KH']^{-1}$. One verification employs the properties (2.3b) and (3.12) of the "true C," whose existence is shown in Lemma 2, to check that using the indicated formula in the upper left block in M^{-1} does in fact lead to $MM^{-1} = I$. Another formula not requiring knowledge of H, and verifiable using (3.12b) and its consequence $(A + KK')^{-1}K = H(K'H)^{-1}$, is $C = (A + KK')^{-1} - (A + KK')^{-1}KK'(A + KK')^{-1}$.

LEMMA 2. *Let* A, K, M *be as in Lemma* 1 *and assume* M *nonsingular. Then there is a unique* p×p *symmetric matrix* C *associated to* K, *with the property that for at least one* H *obeying* (2.2),

$$\text{(a)}\quad K'C=0 \qquad\qquad (2.3)$$
$$\text{(b)}\quad AC=I-K(H'K)^{-1}H'.$$

Furthermore C *obeys* (2.3b) *for every* H *satisfying* (2.2), *and has the additional properties.*

$$\text{(a)}\quad C=CAC,\qquad A=ACA \qquad\qquad (2.4)$$
$$\text{(b)}\quad C \textit{ is of rank } q.$$

PROOF. For any H obeying $H'A=0$ and $\det(H'K)\neq 0$, it is easily verified that any symmetric $p\times p$ matrix C satisfying (2.3) must be a block of M^{-1} placed as in the formula for M^{-1} given in Lemma 1. Furthermore, such a C *does* satisfy (2.3). Since M depends only on K (i.e., not on the choice of H), the same is true of M^{-1} and therefore of C. Since $CK=0$, premultiplication of (2.3b) by C yields $CAC=C$, which implies that the rank of C is at most that of A. Since $H'A=0$, postmultiplication of (2.3b) by A yields $ACA=A$, which implies that the rank of A is at most that of C. Thus (2.4) is proved.[5a]

It is interesting to observe, from eqs (2.2) through (2.4), that the relationship between the pairs (A, H) and (C, K) is symmetric. Also, property (2.4a) shows that C enjoys properties (2.1a) and (2.1b) of A^+. Since A and C are symmetric, (2.1c) and (2.1d) read

$$AC=CA. \qquad (2.5)$$

This will certainly hold (by (2.3b)) if $K=H$, an allowable choice of K in accordance with (2.2) since $\det(H'H)\neq 0$ if $H(p\times r)$ is of rank r. Equation (2.5) will not hold in general,[6] but we shall not require it and so can permit ourselves the freedom of choosing K different from H. The case $q=p$ (i.e., A nonsingular) can be included by appropriate formal conventions concerning "vacuous blocks" in the block matrix M and its inverse; this will be assumed done wherever appropriate, the result (by (2.4a)) being of course $C=A^{-1}$.

The next lemma and its use in the following theorem are not strictly necessary for our purposes, but are included to round out the theory.

LEMMA 3. *Let* A *be a symmetric* p×p *matrix. Then every symmetric* p×p *matrix* C *related to* A *by* (2.4a) *arises from some* K *as above.*

PROOF. Let q and r be as above, and let H be any $p\times r$ matrix of rank r such that $H'A=0$. Let $K(p\times r)$ consist of r columns of $I-AC$ in the same positions as r independent columns of H'. Since $H'(I-AC)=H'$, it follows that $H'K$ is nonsingular and thus that K has rank r. Also since $C(I-AC)=0$, it follows that $CK=0$ and therefore $K'C=0$. To verify (2.3b), first observe that (2.4a) implies (2.4b), so that the equation $C(I-AC)=0$ proves $I-AC$ to have rank not exceeding $p-q=r$. Thus the columns of $I-AC$ not in K are linear combinations of the columns of K, i.e., we can write

$$I-AC=KE$$

for some $r\times p$ matrix E. Then

$$H'=H'(I-AC)=H'KE$$

so that

$$(H'K)^{-1}H'=E$$

and therefore

$$I-AC=K(H'K)^{-1}H',$$

completing the proof.

Now let X be a $p\times n$ matrix. A *weak generalized inverse* of X is an $n\times p$ matrix X^- with the first three of properties (2.1), i.e.,

$$\text{(a)}\quad XX^-X=X$$
$$\text{(b)}\quad X^-XX^-=X^- \qquad\qquad (2.6)$$
$$\text{(c)}\quad (X^-X)'=X^-X.$$

The following theorem, which characterizes the class of all weak generalized inverses of X, in particular establishes the existence of at least one such inverse.

THEOREM. *Let* X *be a* p×n *matrix. The* n×p *matrix* X⁻ *is a weak generalized inverse of* X, *if and only if*

$$X^-=X'C$$

for some C *associated to* A = XX′ *as in Lemma* 2.

PROOF. First suppose $X^-=X'C$ with C associated to A as above. Property (2.6a) reads $ACX=X$, and follows from (2.3b) upon noting that $H'AH=0$ implies [7] $H'X=0$. Property (2.6b) reads $X'CAC=X'C$ and follows from (2.4a), while (2.6c) asserts the symmetry of $X'CX$ and is a consequence of the symmetry of C. To prove the converse, assume X^- is any $n\times p$ matrix obeying (2.6). By (2.6b) and (2.6c),

$$X^-=(X^-X)X^-=X'[(X^-)'X^-].$$

By Lemma 3, it suffices to prove that $C=(X^-)'X^-$ obeys (2.4a). This follows from

$$CAC=(X^-)'X^-X(X^-X)'X^-=(X^-)'X^-XX^-XX^-$$
$$=(X^-)'X^-XX^-=(X^-)'X^-=C,$$
$$ACA=X(X^-X)'X^-XX'=XX^-XX^-XX'$$
$$=XX^-XX'=XX'=A.$$

[5a] From the last formula in footnote 5, we see that C is determined by K only *via* KK'; e.g. C is unchanged if K is replaced by some $(p\times r)$ KL with $LL'=I$.

[6] For a specific example in which eq (2.5) fails, take the rows of A to be (1, 0) and (0, 0), $H'=(0, 1)$, $K'=(1, 1)$; the rows of C are $(1, -1)$ and $(-1, 1)$.

[7] The last equation implies that the sum of the squares of the entries in each row of $H'X$ vanishes.

We note in passing that with $X^- = X'C$, X^- obeys (2.1d) if and only if eq (2.5) holds. Thus (2.1d) holds if the choice $K = H$ is made (this completes the proof that X has a generalized inverse X^+), but as mentioned earlier we shall not have to impose this requirement.

In what follows the notations H, K, C, X^- will have the same significance as in this section, A will stand for XX', and the notation X^+ will be reserved for the generalized inverse. Note that X^- and C need not be uniquely determined by X (although X^+ is), but depend on the choice of K. The relations

$$ACX = X \tag{2.7}$$

$$H'X = 0 \tag{2.8}$$

obtained in connection with the last proof are recorded here for subsequent reference.

3. Fundamental Gauss Theorem for Linear Estimation

The methods of least squares have been in use now for over 150 years. Gauss [1873] in 1821 (collected works 1873) is now credited with placing the method on a sound theoretical basis without any assumptions that the random variables follow a normal distribution. Gauss's contribution was for a time neglected until Markov [1912] "rediscovered" the work of Gauss. It should be noted that Legendre [1806] in 1806 was the first to publish the method of least squares, although apparently Gauss had known about it some years previous. For a more detailed historical introduction consult Merriman [1877], Plackett [1949], and Eisenhart [1964].

In this section we apply the properties of the weak generalized inverse to obtain a proof of the Gauss theorem. The relevance of the generalized inverse to the theory of least squares has been noted by Bjerhammar [1951], Greville [1960], and Penrose [1956]. The fundamental result used in these papers is that for an over-determined system of linear equations

$$X'b = y,$$

$$y' = (y_1, y_2, \ldots, y_n), b' = (b_1, b_2, \ldots, b_p),$$

the selection of b which minimizes the sum of squares of residuals, $(y - X'b)'(y - X'b)$, is given by

$$b = (X')^+ y$$

where $(X')^+$ is the generalized inverse of X'. It is easily verified using (2.1) that $(X')^+ = (X^+)'$, so that by (2.1a) and (2.1c)

$$Ab = XX'(X^+)'y = X(X^+X)'y = (XX^+X)y = Xy$$

i.e., b must be a solution of the usual normal equations $Ab = Xy$ of least-squares theory. More recently Rao [1962] has used property (2.4a) to demonstrate some of the well-known results associated with minimum variance linear unbiased estimation.

Before stating the theorem we review the central idea of an estimable parameter, cf. Bose [1944]. Let $Y' = (Y_1, \ldots, Y_n)$ be a vector of random variables having a distribution which depends on a parameter θ. A function $g(Y)$ of the random vector Y is called an *unbiased estimate of* θ if $E[g(Y)] = \theta$, for all values of θ, where this last phrase may reflect limitations on the possible values of θ imposed by the problem at hand. The parameter θ is called *estimable* if it has at least one unbiased estimate of some form prescribed by the context. In this paper we deal only with *linear* estimates

$$g(Y) = d'Y + c$$

where $d' = (d_1, \ldots, d_n)$ is a $1 \times n$ vector and c is a scalar. A *best* (unbiased linear) estimate of θ is one which has minimum variance among the class of unbiased linear estimates of θ.

THEOREM 1: (Gauss). *Let* X *be a* $p \times n$ *matrix* $(p \leqslant n)$ *of known constants having rank* q, β *a* $p \times 1$ *vector of unknown parameters, and* Y *an* $n \times 1$ *vector of random variables such that*[8]

$$\begin{aligned} E(Y) &= X'\beta \\ \operatorname{var}(Y) &= \sigma^2 I. \end{aligned} \tag{3.1}$$

The minimum variance unbiased linear estimate of any estimable linear function $\theta = l'\beta$ *of* β *(where* l *is a* $p \times 1$ *vector) is*

$$\hat{\theta} = l'(X^-)'Y = l'CXY.$$

For all such θ, $\hat{\theta}$ *can be obtained as* $l'\hat{\beta}$ *where* $\hat{\beta}$ *(independent of* l*) is any vector minimizing the quadratic form* $(Y - X'\beta)'(Y - X'\beta)$, *or equivalently is any solution of the normal equations*

$$A\hat{\beta} = XY \qquad (A = XX') \tag{3.2}$$

whose general solution can be written

$$\hat{\beta} = CXY + (I - CA)z \tag{3.3}$$

with z *an arbitrary* $p \times 1$ *vector.*

PROOF: Let d be an $n \times 1$ vector. Then we remark that the unbiased linear estimates of $\theta = l'\beta$ are precisely the linear forms $d'Y$ with d obeying

$$Xd = l, \tag{3.4}$$

so that θ is estimable if and only if (3.4) has a solution d. Indeed, the function $d'Y + c$ is an unbiased estimate of θ if and only if, for all values of θ,

$$\begin{aligned} l'\beta = \theta &= E(d'Y + c) \\ &= d'E(Y) + c = d'X'\beta + c. \end{aligned}$$

[8] If $Y' = (Y_1, \ldots, Y_n)$, then $E(Y)$ is the vector with $E(Y_k)$ as kth component, and $\operatorname{var}(Y)$ is the $n \times n$ matrix with $\operatorname{cov}(Y_i, Y_j)$ as i, jth entry.

Whether $l=0$ (so that 0 is the only value of θ) or $l\neq 0$ (so that θ assumes all real values), this will be true if and only if $c=0$ and d obeys the system (3.4).

The key idea is to seek a linear change of (random) variable from Y to $\hat{\beta}=B'Y$, where B is an $n\times p$ matrix so chosen that for each estimable $\theta=l'\beta$, at least one unbiased linear estimate of θ can be written in the form $l'\hat{\beta}$. That is, for at least one d_l obeying (3.4) the identity

$$l'B'Y=l'\hat{\beta}=d_l'Y$$

is to hold, or equivalently[9] $d_l=Bl$. For any pair of vectors l and d related by (3.4) we would have

$$Xd=l=Xd_l=XBl=XBXd,$$

and since every d is related to some l by (3.4) (just define l by (3.4)) the equality between the end terms of the last display is an identity in d. This shows that B must be chosen to obey

$$X=XBX. \tag{3.5}$$

Conversely if (3.5) holds then for each d and l related by (3.4) we can set $d_l=BXd$ so that

$$Bl=BXd=d_l \text{ and } Xd_l=XBXd=Xd=l$$

as desired. Therefore (3.5) is exactly the desired relationship, and its resemblance to (2.6a) suggests our setting $B=X^-$ so that

$$d_l=X^-l=X'Cl.$$

The variance of $\hat{\theta}=d'Y$ is $\mathrm{var}(\hat{\theta})=(d'd)\sigma^2$, which is to be minimized by a proper choice of d subject to (3.4). Define an unknown $n\times 1$ vector δ by $d=d_l+\delta$, so that

$$d'd=d_l'd_l+d_l'\delta+\delta'd_l+\delta'\delta.$$

However, since d_l satisfies (3.4) we have

$$d_l'\delta=l'CX(d-X'Cl)=l'Cl-l'CACl=0,$$

so that

$$\mathrm{var}(\hat{\theta})=(d_l'd_l+\delta'\delta)\sigma^2,$$

which is minimized if and only if $\delta=0$, i.e., $d=d_l$. (Incidentally this shows d_l independent of the choice $B=X^-$.) Thus the unique "best estimate" is

$$\hat{\theta}=d_l'Y=l'CXY \tag{3.6}$$

and its variance is

$$\mathrm{var}\,(\hat{\theta})=(d_l'd_l)\sigma^2=(l'CXX'Cl)\sigma^2=l'Cl\sigma^2. \tag{3.7}$$

We have shown that $l'\hat{\beta}$ is a best estimate of θ if and only if

$$l'\hat{\beta}=l'CXY,$$

which, since $l=Xd_l=ACl$, is equivalent to

$$l'C(A\hat{\beta}-XY)=0. \tag{3.8}$$

This shows that any solution $\hat{\beta}$ of the normal equation $A\hat{\beta}=XY$ yields a best estimate $l'\hat{\beta}$ of θ. Conversely[10] if (3.8) is to hold for *all* estimable $\theta=l'\beta$ (i.e. for all l such that (3.4) has a solution d), then since every d is related to some l by (3.4) we have

$$d'X'CA\hat{\beta}=d'X'CXY$$

as an identity in d, so that $X'CA\hat{\beta}=X'CXY$ and premultiplication by X (together with (2.4a) and (2.7)) shows that $\hat{\beta}$ must be a solution of the normal equations.

Since CXY is a solution of the normal equations, the general solution can be written

$$\hat{\beta}=CXY+\eta$$

where η is an arbitrary $p\times 1$ vector such that $A\eta=0$. For any $p\times 1$ vector z,

$$\eta=(I-CA)z$$

satisfies this condition by (2.4a), while conversely any η obeying $A\eta=0$ has the form $(I-CA)z$ with $z=\eta$.

It only remains to show that the solutions $\hat{\beta}$ of the normal equations are precisely the vectors β which minimize the quadratic form

$$Q=(Y-X'\beta)'(Y-X'\beta).$$

For this purpose set $\beta=\hat{\beta}+\delta$ and observe $X(Y-X'\hat{\beta})=0$, so that

$$Q=(Y-X'\hat{\beta})'(Y-X'\hat{\beta})+(X'\delta)'(X'\delta)\geqslant(Y-X'\hat{\beta})'(Y-X'\hat{\beta})$$

where equality holds if and only if $X'\delta=0$ and thus[10a] if and only if $A\delta=0$, i.e., if and only if β (as well as $\hat{\beta}$) satisfies the normal equations.

The preceding analysis essentially contains the description of the class of estimable functions. We rephrase this in the following corollary.[11]

COROLLARY 1.1: *The parametric function $\theta=l'\beta$ is estimable if and only if*

$$(I-AC)l=0 \tag{3.9}$$

or equivalently

$$H'l=0.$$

PROOF. We know that θ is estimable if and only if there exists a vector $d_l=X'Cl$ with $Xd_l=l$. Substi-

[9] We assume for this motivation that the distribution of Y is not concentrated on some lower dimensional subset of n-dimensional space.

[10] This converse, which makes the role of the normal equations precise, was not explicitly stated as part of the theorem.

[10a] Clearly $X'\delta=0$ implies $A\delta=XX'\delta=0$; conversely $XX'\delta=0$ implies $(X'\delta)'(X'\delta)=0$ and thus $X'\delta=0$.

[11] We again remind the reader that H and K are assumed chosen as in section 2, i.e., obeying (2.2).

tuting (2.3b) yields

$$l - Xd_l = (I - AC)l = 0 = K(H'K)^{-1}H'l$$

which implies

$$H'l = 0$$

as desired. Conversely if $(I - AC)l = 0$ then

$$l = ACl = Xd_l \quad (d_l = X'Cl)$$

and if $H'l = 0$ then by (2.3b), $(I - AC)l = 0$ as well.

We observe in particular that the components of $\hat{\beta}$ are best estimates of the corresponding components of β if and only if these components are in fact estimable; by (3.4) this requires that every unit $p \times 1$ vector, and thus every $p \times 1$ vector, be a linear combination of the columns of X. In other words "$\hat{\beta}$ is an estimate of β" makes sense only in the special case $q = p$, when $C = A^{-1}$.

The next corollary pertains to finding a solution of the normal equations by adjoining "dummy" quantities to obtain a system of full rank.

COROLLARY 1.2: *Let* λ *and* m *be* $r \times 1$ *vectors of constants where* m *is arbitrary. Then the unique solution of the system of* $(p + r)$ *simultaneous linear equations*

$$\begin{bmatrix} A & K \\ K' & 0 \end{bmatrix} \begin{bmatrix} \hat{\beta} \\ \lambda \end{bmatrix} = \begin{bmatrix} XY \\ m \end{bmatrix} \tag{3.10}$$

yields a solution of the normal equations; the same holds for the unique solution of the system

$$(A + HK')\hat{\beta} = XY + Hm. \tag{3.11}$$

PROOF. The system (3.10) is of full rank since its coefficient matrix is the M of Lemma 1 in section 2. Therefore the solution can be written

$$\begin{bmatrix} \hat{\beta} \\ \lambda \end{bmatrix} = \begin{bmatrix} C & H(K'H)^{-1} \\ (H'K)^{-1}H' & 0 \end{bmatrix} \begin{bmatrix} XY \\ m \end{bmatrix} = \begin{bmatrix} CXY + H(K'H)^{-1}m \\ (H'K)^{-1}H'XY \end{bmatrix}. \tag{3.11a}$$

However since $H'X = 0$, the vector λ is identically zero. Since K has rank r, m can be written as $K'z$ where z is a $p \times 1$ vector; then the solution vector $\hat{\beta}$ is $\hat{\beta} = CXY + (I - CA)z$ which is the general solution of the normal equations. It also follows that the $\hat{\beta}$ of (3.10)'s solution satisfies (3.11), since $K'\hat{\beta} = m$. It only remains to prove that (3.11)'s solution is unique, i.e., that $A + HK'$ is nonsingular. This is true since it can be directly verified using (2.3b), (2.3a), and (2.8) that

$$(A + HK')^{-1} = C + [H(K'H)^{-1} - CH](H'H)^{-1}H'. \tag{3.12}$$

For situations in which a suitable K is known but a suitable H is not at hand, it may be desirable to replace (3.11) by an analogous system not involving H. Such a system is given by

$$(A + KK')\hat{\beta} = XY + Km, \tag{3.12a}$$

which is satisfied by the $\hat{\beta}$ of (3.10)'s solution, and which has only one solution since

$$(A + KK')^{-1} = C + H(K'H)^{-1}(H'K)^{-1}H' \tag{3.12b}$$

as can be directly verified using (2.3). Lacking H, one might still want to know C in order to check estimability by (3.9).

From the criterion (3.9) and the fact that K is of rank r, it follows that the elements of $K'\beta$ are an independent set of nonestimable functions with the additional property that $[A, K]$ has independent rows. The analysis of (3.10), together with the Gauss theorem, shows that the values of these nonestimable linear functions can be prescribed in any way (i.e., $K'\beta = m$) without affecting the best estimates of the estimable functions; $\hat{\beta}$ depends on m but $\hat{\theta} = l'\hat{\beta}$ (where $\theta = l'\beta$ is estimable) does not. The results of prescribing (in a self-consistent way) the values of an arbitrary set of linear forms in β are treated in section 4.

It is natural to inquire as to the significance of $l'\hat{\beta}$ when $\theta = l'\beta$ is *not* necessarily estimable. One form of the answer is given in the next corollary.

COROLLARY 1.3: *Let* $\hat{\beta} = CXY$. *Then for any* $\theta = l'\beta$, *there is a unique* [11a] *estimable function* $\theta_1 = l_1'\beta$, *namely* $\theta_1 = l'CA\beta$, *such that* $l\hat{\beta}$ *is the best estimate of* θ_1.

PROOF. First assume $l_1 = ACl$ and $\theta_1 = l_1'\beta$, so that θ_1 is estimable by Corollary 1.1. Then the Gauss theorem implies that $l'\hat{\beta}$ is the best estimate of θ_1, since by (2.4)

$$l'\hat{\beta} = l'CXY = l'CACXY$$
$$= (ACl)'CXY = l_1'\hat{\beta}.$$

To prove the uniqueness of θ_1, consider *any* estimable $\theta_1 = l_1'\beta$ such that $l'\hat{\beta}$ is the best estimate of θ_1. Then by Corollary 1.1 $H'l_1 = 0$, so that $l_1 = A\eta$ for some $p \times 1$ vector η. Also we must have

$$l'CXY = l'\hat{\beta} = l_1'\hat{\beta} = \eta'ACXY = \eta'XY,$$

so that $X'Cl = X'\eta$ and therefore

$$l_1 = XX'\eta = XX'Cl = ACl$$

as asserted.

For completeness we include some known facts about the vector of residuals

$$\delta = Y - X'\hat{\beta}$$

(where $\hat{\beta}$ is any solution of the normal equations [12]) and

[11a] The uniqueness assertion requires the assumption mentioned in footnote 9. Note that a definite choice of C is assumed.

[12] Note that δ is independent of the choice of $\hat{\beta}$.

the usefulness in estimating σ^2 of its squared length (the residual sum of squares)

$$S^2=\delta'\delta=(Y-X'\hat{\beta})'(Y-X'\hat{\beta})=Y'Y-\hat{\beta}'A\hat{\beta}.$$

COROLLARY 1.4: *The residual vector is uncorrelated with the estimate of any estimable function; in fact* [12a]

$$\mathrm{Cov}(\hat{\beta},\delta)=0.$$

Furthermore we have

$$\mathrm{E}(S^2)=(n-q)\sigma^2.$$

PROOF. The expected value of the residual vector is

$$E(\delta)=E(Y)-E(X'\hat{\beta})=0.$$

Therefore

$$\begin{aligned}\mathrm{Cov}(\hat{\beta},\delta)&=E\{\hat{\beta}\delta'\}-E\{E(\hat{\beta})\delta'\}\\&=E\{[CXY][Y-X'\hat{\beta}]'\}=CXE(YY')(I-X'CX).\end{aligned}$$

Since

$$E(YY')=\sigma^2I+(X'\beta)(X'\beta)'$$

we have

$$\begin{aligned}\mathrm{Cov}(\hat{\beta},\delta)&=CX[\sigma^2I+X'\beta\beta'X][I-X'CX]\\&=C[\sigma^2I+A\beta\beta'][X-ACX]=0\end{aligned}$$

because $X=ACX$ from (2.7).

To prove the second assertion we use the general formula

$$E(Y'BY)=E(Y')BE(Y)+\mathrm{trace}\,(B\ \mathrm{var}\,(Y))$$

for the mean of a quadratic form, with

$$B=(I-X'CX)^2=I-X'CX,$$

to obtain

$$\begin{aligned}E(S^2)&=E(\delta'\delta)\\&=\beta'X(I-X'CX)X'\beta+\sigma^2\ \mathrm{trace}\,(I-X'CX)\\&=\sigma^2\ \mathrm{trace}\,(I-X'CX)\\&=\sigma^2[n-\mathrm{trace}\,(X'CX)].\end{aligned}$$

By the general formula trace $(M_1M_2')=$ trace $(M_2'M_1)$ where M_1 and M_2 are rectangular matrices of the same dimensions, we have

$$\begin{aligned}\mathrm{trace}\,(X'CX)&=\mathrm{trace}\,(XX'C)=\mathrm{trace}\,(AC)\\&=\mathrm{trace}\,(I-K(H'K)^{-1}H')\\&=p-\mathrm{trace}\,[(H'K)(H'K)^{-1}]\\&=p-r=q,\end{aligned}$$

completing the proof.

A final comment deals with the maximum possible number of linearly independent nonestimable parametric functions $\theta=l'\beta$. If $q=p$ (i.e., A is nonsingular) then this number is *zero*; every linear function of β is estimable since β itself is estimable (see the remarks after Corollary 1.1). If $q<p$, however, then the number is p rather than r (as is occasionally suggested). This can be seen by partitioning $A=[A_1, A_2]$, where A_1 consists of q independent columns of A. Then the $p\times p$ matrix $[H, A_1]$ is nonsingular, since $H'H$ and $A_1'A_1$ are nonsingular and

$$\begin{bmatrix}(H'H)^{-1}H'\\(A_1'A_1)^{-1}A_1'\end{bmatrix}[H, A_1]=I.$$

Therefore, if h is a column of H and $\alpha_1, \alpha_2, \ldots \alpha_q$ are the columns of A_1, then

$$N=[H, \alpha_1+h, \alpha_2+h, \ldots, \alpha_q+h]$$

has the same determinant as $[H, A_1]$ and so is also nonsingular. The p columns of N are therefore the vectors "l" of coefficients of p independent parametric functions, which are all nonestimable since the nonsingularity of $H'H$ implies that no column of

$$H'N=[H'H, H'h, H'h, \ldots, H'h]$$

is the zero vector.

4. Gauss Theorem With Given Restraints

Often experimental situations arise in which the parameters (components of β) are connected by known linear relations. It is not generally realized that some of the linear forms whose values are prescribed by these given restraints may be estimable with respect to the equations of condition $E(Y)=X'\beta$ where as before we assume X is $p\times n$ ($p\leq n$) and of rank q. In this section we discuss the appropriate extension of the Gauss theorem when these equations of condition are supplemented by known linear constraints. It will be shown that several applications of the "simple" Gauss theorem of section 3 suffice to reduce such problems to purely matrix-theoretic questions.

We introduce the term *pre-estimable* to be used in this section for those parametric functions (linear in β) which are estimable with respect to $E(Y)=X'\beta$. The term estimable will refer to the parametric functions which are estimable with all the given information including the restraints. Clearly every pre-estimable parameter is also estimable, but the converse need not hold; for example a nonpre-estimable function whose value is specified by one of the given constraints is obviously estimable.

We will find it convenient to assume that the constraints have been brought into an "irreducible form" in a sense made precise in this and the next few

[12a] By definition, $\mathrm{Cov}(\hat{\beta},\delta)$ is the matrix $E\{[\hat{\beta}-E(\hat{\beta})][\delta-E(\delta)]'\}$.

paragraphs. Suppose the initially given restraints are

$$L'\beta = \bar{m}$$

where L' is $k \times p$ with rank k, and $\bar{m}$ is $k \times 1$. The matrix L can be partioned into $L=(L_1, L_2)$ where L_i is $p \times s_i$ $(k = s_1 + s_2)$ with rank s_i such that $L_1'\beta = \bar{m}_1$ is nonpre-estimable and $L_2'\beta = \bar{m}_2$ is pre-estimable; i.e., $H'L_1$ has no zero column and $H'L_2 = 0$. Since H has rank $r = p - q$, we know that $s_2 \leq q$. Furthermore from the remarks at the end of section 3, the maximum number of linearly independent nonpre-estimable restraints [13] is p; hence $s_1 \leq p$.

Let the rank of the $r \times s_1$ matrix $H'L_1$ be ν. There will then exist a $s_1 \times (s_1 - \nu)$ matrix G with rank $s_1 - \nu$ such that $H'L_1G = 0$. Also there will exist a $s_1 \times \nu$ matrix F with rank ν such that $F'G = 0$. We can for example take F' to consist of ν linearly independent rows of $H'L_1$. Then the square matrix of order s_1, $S = (F, G)$, has rank s_1. Hence we can premultiply the nonpre-estimable restraints $L_1'\beta$ by S' to obtain [14]

$$\begin{bmatrix} F' \\ G' \end{bmatrix} L_1'\beta = \begin{bmatrix} F'L_1'\beta \\ G'L_1'\beta \end{bmatrix} = \begin{bmatrix} F'\bar{m}_1 \\ G'\bar{m}_1 \end{bmatrix}.$$

Since $H'L_1G = 0$, the $(s_1 - \nu)$ restraints $G'L_1'\beta$ are pre-estimable. It is clear that the restraints $F'L_1'\beta$ are nonpre-estimable, as $H'L_1F$ has no zero column by virtue of $F'G = 0$. Thus the original k restraints $L'\beta = \bar{m}$ may be regarded as being transformed into two sets

$$K_1'\beta = m_1, \qquad m_1 = F'\bar{m}_1$$

$$K_2'\beta = m_2, \qquad m_2 = \begin{bmatrix} G'\bar{m}_1 \\ \bar{m}_2 \end{bmatrix}$$

where K_i is $p \times k_i$ with rank k_i such that

$$K_1' = F'L_1', \; k_1 = \nu$$

$$K_2' = \begin{bmatrix} G'L_1' \\ L_2' \end{bmatrix}, \; k_2 = (s_1 - \nu) + s_2$$

with $H'K_2 = 0$. Furthermore the rank of the $r \times k_1$ matrix $H'K_1 = H'L_1F$ $(k_1 < p)$ is [14a] k_1 and hence the rank of K_1 is also k_1.

When the given s_1 nonpre-estimable restraints $L_1'\beta$ are such that the rank ν of $H'L_1$ is s_1 (equal to the number of nonpre-estimable restraints) then these restraints will be termed *irreducible* restraints. Alternatively if the rank ν of $H'L_1$ is $< s_1$ (smaller than the number of nonpre-estimable restraints) the restraints $L_1'\beta$ will be called *reducible* restraints since it is then possible (as was just shown) to obtain pre-estimable restraints from them. Unless otherwise indicated the given restraints in this section will be denoted by

$$\begin{bmatrix} K_1'\beta \\ K_2'\beta \end{bmatrix} = \begin{bmatrix} m_1 \\ m_2 \end{bmatrix}$$

where K_i is $p \times k_i$ and has rank k_i. Furthermore the restraints $K_1'\beta$ are a set of k_1 irreducible nonpre-estimable restraints and $K_2'\beta$ denotes a set of k_2 pre-estimable restraints; i.e., $H'K_2 = 0$. Since k_1 and r are the ranks of $H'K_1$ and H respectively, we must have $k_1 \leq r$.

THEOREM 2. *Let* X, β, *and* Y *be as before, satisfying*

$$\mathrm{E}(\mathrm{Y}) = \mathrm{X}'\beta, \; \mathrm{var}\, \mathrm{Y} = \sigma^2 \mathrm{I}.$$

Also let there be given known linear restraints among the parameters of the form

$$\mathrm{K}_1'\beta = \mathrm{m}_1, \; \mathrm{K}_2'\beta = \mathrm{m}_2$$

where K_i *is* $\mathrm{p} \times \mathrm{k}_i$ *with rank* k_i *and* m_i *is* $\mathrm{k}_i \times 1$. *The* k_1 *restraints* $\mathrm{K}_1'\beta = \mathrm{m}_1$ *are irreducible and nonpre-estimable whereas the* k_2 *restraints* $\mathrm{K}_2'\beta = \mathrm{m}_2$ *are pre-estimable. With* H *as before, let* $\mathrm{H} = [\mathrm{H}_0, \mathrm{H}_1]$ *correspond to a partition such that* H_0 *is* $\mathrm{p} \times (\mathrm{r} - \mathrm{k}_1)$ *and* H_1 *is* $\mathrm{p} \times \mathrm{k}_1$ *where* $\det \mathrm{H}_1'\mathrm{K}_1 \neq 0$. *Then the minimum variance linear unbiased estimate of the estimable function* $\theta = l'\beta$ *is*

$$\hat{\theta} = l'\{\mathrm{CXY} + \mathrm{H}_1(\mathrm{K}_1'\mathrm{H}_1)^{-1}\mathrm{m}_1 + \mathrm{CK}_2(\mathrm{K}_2'\mathrm{CK}_2)^{-1}(\mathrm{m}_2 - \mathrm{K}_2'\mathrm{CXY})\}$$

where the matrix C *is obtained from Lemma 2 with* K *taken to be* $\mathrm{K} = [\mathrm{K}_0, \mathrm{K}_1]$ *and* $\mathrm{K}_0(\mathrm{p} \times (r - \mathrm{k}_1))$ *chosen such that* $\det \mathrm{H}'\mathrm{K} \neq 0$.

PROOF. [14b] A partition $H = [H_0, H_1]$ with the desired properties can be formed by taking H_1' to consist of k_1 rows of H' in the same positions as k_1 linearly independent rows of $H'K_1$. We first show that the unbiased linear estimates of $\theta = l'\beta$ are precisely the linear forms

$$g(Y) = d'Y + d_1'm_1 + d_2'm_2, \tag{4.1}$$

for which

$$Xd + K_1d_1 + K_2d_2 = l, \tag{4.2}$$

where d is an $n \times 1$ vector and d_i is a $k_i \times 1$ vector. Thus θ is estimable if and only if (4.2) has a solution $[d', d_1', d_2']$. The proof is based on the observation that

$$Z' = [Y', m_1', m_2']$$

defines an $(n + k_1 + k_2) \times 1$ random vector Z (recall

[13] We will use the term "restraint" to refer to a constrained linear form as well as to the constraint equation itself.

[14] Since S is nonsingular, $L'\beta = \bar{m}_1$ is logically equivalent to $S'L_1'\beta = S'\bar{m}_1$.

[14a] For some nonsingular $\nu \times \nu$ matrix U, we have $F = \bar{F}U$ where $\bar{F}(r \times s_1)$ consists of $\nu = k_1$ independent rows of $H'L_1$. Also $L_2'H = \bar{F}P$, where P is a $k_1 \times r$ matrix of rank k_1. Then $K_1'H = F'L_1'H = U'\bar{F}'\bar{F}P$; since $U'\bar{F}'\bar{F}$ is nonsingular, $K_1'H$ is also of rank k_1.

[14b] We point out in advance that rearranging the columns of H and/or K does not alter the properties required of H and K (i.e., (2.2)).

that a constant is a special case of a random variable), and that

$$E(Y)=X'\beta, \qquad K_1'\beta=m_1, \qquad K_2'\beta=m_2$$

are equivalent to $E(Z)=[X, K_1, K_2]'\beta$. Thus the assertion is proved by the proof of (3.4), with Z replacing Y, $[X, K_1, K_2]$ replacing X, and $[d', d_1', d_2']$ replacing d'.

The nonsingularity of $H_1'K_1$ can be used to solve (4.2) for d_1 after premultiplying it by H_1'. The result is

$$d_1=(H_1'K_1)^{-1}H_1'l,$$

so that the unbiased linear estimates of $\theta=l'\beta$ are precisely the linear forms

$$g(Y)=d'Y+d_2'm_2+l'H_1(K_1'H_1)^{-1}m_1 \tag{4.3}$$

for which

$$Xd+K_2d_2=[I-K_1(H_1'K_1)^{-1}H_1']l=l^*. \tag{4.4}$$

Thus θ is estimable if and only if (4.4) has a solution $[d', d_2']$.

Since $\text{var}\,[g(Y)]=\text{var}\,(d'Y)=\sigma^2d'd$, as before (in section 3) the objective is to minimize $d'd$, but now the side condition on d is the existence of a d_2 related to d by (4.4). Initially regard d_2 as fixed; then the minimization of $d'd$ subject to $Xd=l^*-K_2d_2$ is identical with the problem of finding a best estimate for $(l^*-K_2d_2)'\beta$ subject to (3.1). By the Gauss theorem of section 3, the unique solution (as a function of d_2) is

$$d=X'C(l^*-K_2d_2)=X'C\{[I-K_1(H_1'K_1)^{-1}H_1']l-K_2d_2\}. \tag{4.5}$$

In (4.5) the matrix C is obtained from Lemma 2 for *some* appropriate K; choosing [15] K as in the statement of the theorem yields $CK_1=0$ (since C is symmetric and (2.3a) holds); so that (4.5) simplifies to

$$d=X'Cl-X'CK_2d_2. \tag{4.6}$$

This simplification was the purpose for choosing the indicated form $K=[K_0, K_1]$.

Let $Y^*=X'Cl$ and $X^*=K_2'CX$. Then the quadratic form $d'd$ to be minimized becomes, by (4.6),

$$Q^*=(Y^*-(X^*)'d_2)'(Y^*-(X^*)'d_2),$$

and the condition on d_2 is that it be related to some d by (4.4). This condition is, however, automatically satisfied for *any* d_2, which can be seen as follows. First, the estimability of θ implies that l^* can be written in at least one way in the form (4.4), say

$$l^*=X\delta+K_2\delta_2.$$

Second, the pre-estimability of $K_2'\beta$ (i.e.; the fact $H'K_2=0$) implies that $K_2=XB$ for some $n\times k_2$ matrix B. Combining these observations gives (for any d_2)

$$l^*-K_2d_2=X(\delta+B\delta_2-Bd_2)=Xd \qquad (d=\delta+B\delta_2-Bd_2)$$

as desired.

The choices of d_2 (now unrestrained) which minimize Q^* are known by the Gauss theorem to be precisely the vectors

$$d_2=C^*X^*Y^*+(I-C^*A^*)z, \tag{4.7}$$

where z is an arbitrary $k_2\times 1$ vector and C^* is related to

$$A^*=X^*(X^*)'=K_2'CXX'CK_2=K_2'CK_2 \tag{4.8}$$

as C is to A. We shall however show below that $I-A^*C^*=0$, so that A^* is nonsingular and the solution becomes uniquely

$$d_2=(A^*)^{-1}X^*Y^*=(K_2'CK_2)^{-1}K_2'Cl. \tag{4.9}$$

Substitution of (4.6) and (4.9) into (4.3) gives the best estimate $\hat\theta$ as asserted in the statement of the theorem.

Since K_2 has linearly independent columns, we can prove $I=A^*C^*$ by showing that

$$(I-A^*C^*)K_2'=0.$$

For this purpose write $K_2=XB$ as above, and use eq (2.6a) to obtain

$$K_2'=B'(XX^-X)'=B'X'(X^-)'X'=K_2'(X'C)'X'=X^*X'.$$

Then the version $A^*C^*X^*=X^*$ of (2.7) gives

$$(I-A^*C^*)K_2'=(I-A^*C^*)X^*X'=0$$

as desired, completing the proof of the theorem. We shall frequently use the consequence

$$ACK_2=K_2 \tag{4.10}$$

of $K_2=XB$ and $ACX=X$.

COROLLARY 2.1: *The parametric function $\theta=l'\beta$ is estimable if and only if*

$$H_0'[I-K_1(H_1'K_1)^{-1}H_1']l=0. \tag{4.11}$$

Furthermore if H_0 is chosen such that $H_0'K_1=0$, then the condition reduces to

$$H_0'l=0 \tag{4.12}$$

PROOF. The necessary and sufficient condition for θ to be estimable was shown to be (4.4), i.e.,

$$Xd+K_2d_2=[I-K_1(H_1'K_1)^{-1}H_1']l \tag{4.13}$$

holds for some d and d_2. Since $H_0'X=0$ and $H_0'K_2=0$, eq (4.11) holds. Conversely if (4.11) holds, then

$$H'[I-K_1(H_1'K_1)^{-1}H_1']l=0$$

[15] To show that such a choice is possible in at least one way, select any $p\times(r-k_1)$ matrix K_0 of rank $r-k_1$ such that $H_1'K_0=0$ and $AK_0=0$. If $H_0=K_0$ held, then (2.2a) would be satisfied and

$$H'K=[H_0, H_1]'[K_0, K_1]$$

would have nonsingular square blocks $H_0'H_0$ and $H_1'K_1$ on its main diagonal, implying the desired relation $\det(H'K)\neq 0$. Since by Lemma 1 this relation (for fixed K) is independent of the particular choice of H, it persists even if $H_0\neq K_0$.

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which implies that (4.13) holds for some d and d_2, which in turn means that $\theta = l'\beta$ is estimable.

The only restrictions on $H = [H_0, H_1]$ and $K = [K_0, K_1]$ are that $H'K \neq 0$, $H'A = 0$, $\det H_1'K_1 \neq 0$ and that both H and K have rank $r = p - q$. The matrix H_0 can be chosen in any way subject to satisfying the above conditions. H_0 can always be taken to satisfy $H_0'K_1 = 0$ by taking an initial $\tilde{H}_0$ for which the above conditions hold and letting

$$H_0 = [I - H_1(K_1'H_1)^{-1}K_1']\tilde{H}_0.$$

It is easy to verify that $H_0'A = 0$, and further that $H_0'K_1 = 0$. By Lemma 1, if the matrix $H = [H_0, H_1]$ has rank r, then $\det(H'K) \neq 0$. To prove that H has the required rank r, we write the formula for H_0 as

$$H_0 = \tilde{H}_0 - H_1P \qquad (P = (K_1'H_1)^{-1}K_1'\tilde{H}_0)$$

and observe that

$$[H_0, H_1] = [H_0, H_1]\begin{bmatrix} I & 0 \\ -P & I \end{bmatrix}$$

where the first factor on the right-hand side has rank r while the second is $r \times r$ and nonsingular.

Note that the previous construction did not depend on K_0. We now show, in addition, that K_0 can be so chosen that $H_1'K_0 = 0$. Simply replace an initial $\tilde{K}_0$ by

$$K_0 = [I - K_1(H_1'K_1)^{-1}H_1']\tilde{K}_0;$$

then $H_1'K_0 = 0$, and $H_0'K_0$ has the required rank $r - k_1$ since it coincides with $H_0'\tilde{K}_0$.

For simplicity we shall assume in what follows that H_0' and K_0 are chosen so that both $H_0'K_1 = 0$ and $H_1'K_0 = 0$. Thus the estimability condition is given by $H_0'l = 0$, and the frequently occurring inverse $(H'K)^{-1}$ takes the simple form

$$(H'K)^{-1} = \operatorname{diag}[(H_0'K_0)^{-1}, (H_1'K_1)^{-1}]. \qquad (4.14)$$

Then the general form of the vector $\hat{\beta}$, such that the best estimate of *every* estimable $l'\beta$ is $l'\hat{\beta}$, is given by

$$\hat{\beta} = CXY + H_0(K_0'H_0)^{-1}m_0 + H_1(K_1'H_1)^{-1}m_1 + CK_2(K_2'CK_2)^{-1}(m_2 - K_2'CXY), \qquad (4.15)$$

where m_0 is an arbitrary $(r - k_1) \times 1$ vector.

The next corollary formulates some systems of equations involving "dummy" variables (μ_0, μ_1, λ) and artificial restraints ($K_0'\beta = m_0$) which can be used to solve for $\hat{\beta}$ of (4.15).

COROLLARY 2.2: *Let μ_0 and m_0 be $(r - k_1) \times 1$ vectors, μ_1 a $k_1 \times 1$ vector and λ a $k_2 \times 1$ vector. Then every solution $\hat{\beta}$ of the system*

$$\begin{bmatrix} A & K_2 \\ K_1' & 0 \\ K_2' & 0 \end{bmatrix}\begin{bmatrix} \hat{\beta} \\ \lambda \end{bmatrix} = \begin{bmatrix} XY \\ m_1 \\ m_2 \end{bmatrix} \qquad (4.16)$$

can be used in the best estimate $\theta = l\hat{\beta}$ of any estimable function $\theta = l'\beta$. The same holds for the unique solutions of each of the systems

$$\begin{bmatrix} A & K_0 & K_1 & K_2 \\ K_0' & 0 & 0 & 0 \\ K_1' & 0 & 0 & 0 \\ K_2' & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} \hat{\beta} \\ \mu_0 \\ \mu_1 \\ \lambda \end{bmatrix} = \begin{bmatrix} XY \\ m_0 \\ m_1 \\ m_2 \end{bmatrix}, \qquad (4.17)$$

$$\begin{bmatrix} A & K_2 \\ K_0' & 0 \\ K_1' & 0 \\ K_2' & 0 \end{bmatrix}\begin{bmatrix} \hat{\beta} \\ \lambda \end{bmatrix} = \begin{bmatrix} XY \\ m_0 \\ m_1 \\ m_2 \end{bmatrix} \qquad (4.18)$$

$$\begin{bmatrix} A + H_0K_0' + H_1K_1' & K_2 \\ K_2' & 0 \end{bmatrix}\begin{bmatrix} \hat{\beta} \\ \lambda \end{bmatrix} = \begin{bmatrix} XY + H_0m_0 + H_1m_1 \\ m_2 \end{bmatrix}, \qquad (4.19)$$

as well as the vector

$$\hat{\beta} = \hat{\beta}_0 + CK_2(K_2'CK_2)^{-1}(m_2 - K_2'CXY) \qquad (4.20)$$

where $\hat{\beta}_0$ is obtained from the unique solution of

$$\begin{bmatrix} A & K_0 & K_1 \\ K_0' & 0 & 0 \\ K_1' & 0 & 0 \end{bmatrix}\begin{bmatrix} \hat{\beta}_0 \\ \mu_0 \\ \mu_1 \end{bmatrix} = \begin{bmatrix} XY \\ m_0 \\ m_1 \end{bmatrix}. \qquad (4.21)$$

PROOF. System (4.16) does not have a unique solution for $k_1 < r$, but for any solution $[\hat{\beta}', \lambda']$ we can *define* a vector m_0 by $K_0'\hat{\beta} = m_0$ and observe that $[\hat{\beta}', \lambda']$ satisfies (4.18). Thus the discussion of (4.16) reduces to that of (4.18).

Since the $\hat{\beta}$ of (4.15) clearly obeys $K_i'\hat{\beta} = m_i$, and also (premultiply $\hat{\beta}$ by CA) satisfies

$$C\{A\hat{\beta} + K_2\lambda - XY\} = 0$$

where

$$\lambda = (K_2'CK_2)^{-1}(K_2'CXY - m_2), \qquad (4.22)$$

we find that $\hat{\beta}$ and λ obey (4.18). Thus the solution of (4.18), once it is proved unique, must have the form (4.15).

The first subsystem

$$A\hat{\beta} + K_0\mu_0 + K_1\mu_1 + K_2\mu_2 = XY$$

of (4.17), when premultiplied by $(H_0'K_0)^{-1}H_0'$, yields $\mu_0 = 0$; then premultiplication of

$$A\hat{\beta} + K_1\mu_1 + K_2\mu_2 = XY$$

by $(H_1'K_1)^{-1}H_1'$ yields $\mu_1 = 0$. Thus every solution of

(4.17) is a solution of (4.18), so (4.17) does not require further discussion. Note that the dummy variables μ_0 and μ_1 are zero vectors in the solution.

It is trivial to check that any solution of (4.18) is also a solution of (4.19). Thus the results for (4.16) through (4.19) will be proved once we show that (4.19) has a unique solution. The utility of (4.19) is that it is a smaller system than those preceding it. We write the first subsystem of (4.19) in the form

$$(A+HK')\hat{\beta}=XY+Hm-K_2\lambda$$

where $m'=(m_0', m_1')$. By Corollary 1.2, $A+HK'$ is nonsingular so that $\hat{\beta}$ is directly determined in terms of λ by

$$\hat{\beta}=(A+HK')^{-1}(XY+Hm)-(A+HK')^{-1}K_2\lambda.$$

Corollary 1.2 shows that the first term on the right is just $\hat{\beta}_0$, while since $H'K_2=0$ the formula (3.12) for $(A+HK')^{-1}$ shows that we have

$$\hat{\beta}=\hat{\beta}_0-CK_2\lambda. \tag{4.23}$$

After premultiplying by $(K_2'CK_2)^{-1}K_2'$, noting $K_2'\hat{\beta}=m_2$, we obtain a unique λ.

To treat (4.20) we first use (4.14) to obtain

$$H(K'H)^{-1}=[H_0(K_0'H_0)^{-1}, H_1(K_1'H_1)^{-1}]$$

and then apply corollary 1.1 (see (3.11a)) to the system (4.21) to show that its unique solution has

$$\hat{\beta}_0=CXY+H_0(K_0'H_0)m_0+H_1(K_1'H_1)^{-1}m_1. \tag{4.24}$$

Thus $\hat{\beta}$ given by (4.20) coincides with (4.15).

COROLLARY 2.3. *With the particular choice* $\hat{\beta}=CXY+H_1(K_1'H_1)^{-1}m_1+CK_2(K_2'CK_2)^{-1}(m_2-K_2'CXY)$ *for any* $\theta=l'\beta$ *there is a unique*[15a] *estimable* $\theta_1=l_1'\beta$, *given by* $l_1=[AC+K_1(H_1'K_1)^{-1}H_1']l$ *such that for all possible* m_1, m_2 *and* $\beta, l'\hat{\beta}$ *is the best estimate of* θ_1.

PROOF. First assume $l_1=[AC+K_1(H_1'K_1)^{-1}H_1']l$ and $\theta_1=l_1'\beta$. Then $H_0'l_1=0$, so θ_1 is estimable, and we have

$$l_1'\hat{\beta}=l'[CA+H_1(K_1'H_1)^{-1}K_1']\hat{\beta}=l'\hat{\beta}$$

by direct calculation (using $CAC=C$, $AH_1=0$, $K_1'C=0$) so that $l'\hat{\beta}$ is the best estimate of θ_1. To prove uniqueness, consider any estimable $\theta_1=l_1'\beta$ such that $l'\hat{\beta}$ is the best estimate of θ_1 for all m_1 and m_2. Note with the aid of (2.2a), that $\det(H_1'K_1)\neq 0$ implies that $[A, K_1]$ has rank $q+k_1$. Since $H_0'[A, K_1]=0$ and H_0 has rank $p-(q+k_1)$, it follows from $H_0'l_1=0$ that $l_1=Ad+K_1d_1$ for some vectors d and d_1. Using $ACX=X$ and $ACK_2=K_2$ we obtain

$$l_1'\hat{\beta}=d'[(I-K_2(K_2'CK_2)^{-1}K_2'C)XY + K_2(K_2'CK_2)^{-1}m_2]+d_1'm_1.$$

Setting $m_i=K_i'\beta$ $(i=1, 2)$ and equating the coefficients of Y and β in $l_1'\beta$ and $l'\hat{\beta}$, we obtain

$$X'(I-CK_2(K_2'CK_2)^{-1}K_2')(d-Cl)=0, \tag{4.25}$$

$$K_2(K_2'CK_2)^{-1}K_2'(d-Cl)=K_1[(H_1'K_1)^{-1}H_1'l-d_1] \tag{4.26}$$

Multiplication of the second equation by H_1' leads to $H_1'l=H_1'K_1d_1$ and thus to

$$d_1=(H_1'K_1)^{-1}H_1'l$$

as desired. Substitution of this into (4.26) yields a result which when substituted into (4.25) gives

$$X'(d-Cl)=0$$

implying that $Ad=ACl$ as desired.

We turn now to the residual vector $\delta=Y-X'\hat{\beta}$ and the residual sum of squares $S^2=\delta'\delta$.

COROLLARY 2.4. *The residual sum of squares can be written as*

$$S^2=\delta'\delta=(Y-X'\hat{\beta}_0)'(Y-X'\hat{\beta}_0)+\lambda'(K_2'CK_2)\lambda \tag{4.27}$$

and has the expected value

$$E(S^2)=(n-q+k_2)\sigma^2,$$

where $\hat{\beta}_0$ *is the estimate ignoring the preestimable restraint* $K_2'\beta=m_2$ *and*

$$\lambda=(K_2'CK_2)^{-1}(K_2'CXY-m_2).$$

PROOF. The residual sum of squares can be written

$$S^2=\delta'\delta=(Y-X'\hat{\beta}_0+X'CK_2\lambda)'(Y-X'\hat{\beta}_0+X'CK_2\lambda)$$

$$=(Y-X'\hat{\beta}_0)'(Y-X'\hat{\beta}_0)+\lambda'(K_2'CK_2)\lambda+2(Y-X'\hat{\beta}_0)'X'CK_2\lambda.$$

However we have

$$(Y-X'\hat{\beta}_0)'X'CK_2\lambda=(Y'X'C-\hat{\beta}_0'AC)K_2\lambda$$

$$=(Y'X'C-Y'X'CAC)K_2\lambda=0$$

and thus

$$S^2=(Y-X'\hat{\beta}_0)'(Y-X'\hat{\beta}_0)+\lambda'(K_2'CK_2)\lambda.$$

From Corollary 1.4 of section 3 we have

$$E\{(Y-X'\hat{\beta}_0)'(Y-X'\hat{\beta}_0)\}=(n-q)\sigma^2.$$

Furthermore

$$E(\lambda)=(K_2'CK_2)^{-1}(K_2'\beta-m_2)=0, \text{ var } \lambda=(K_2'CK_2)^{-1}\sigma^2.$$

Making use of the formula for finding the expectation

[15a] The uniqueness assertion requires the assumption mentioned in footnote 9.

of a quadratic form [16] gives

$$E(\lambda' K_2' C K_2 \lambda) = \text{trace}\,\{(K_2' C K_2)(\text{var}\,\lambda)\}$$

$$= \text{trace}\,\{(K_2' C K_2)(K_2' C K_2)^{-1}\sigma^2\} = k_2\sigma^2,$$

and thus the result is proved. Note that the formula for S^2 is composed of two parts, the second of which measures the deviation between the values of the pre-estimable restraints $K_2'\beta$ as estimated from the data (Y), and the given values m_2 of these restraints.

COROLLARY 2.5. *The residual vector* $\delta = Y - X'\hat{\beta}$ *is uncorrelated with any estimable function; in fact*

$$\text{Cov}\,(\delta, \hat{\beta}) = 0. \tag{4.28}$$

PROOF. We write $\delta_0 = Y - X'\hat{\beta}_0$ as the residual vector if the restraints $K_2'\beta = m_2$ had been ignored. By (4.20) $\delta = \delta_0 + X'CK_2\lambda$ and $\hat{\beta} = \hat{\beta}_0 - CK_2\lambda$ and we can write

$$\text{Cov}\,(\delta, \hat{\beta}) = \text{cov}\,(\delta_0, \hat{\beta}_0) - \text{cov}\,(\delta_0, \lambda)K_2'C$$

$$+ X'CK_2\,\text{cov}\,(\lambda, \hat{\beta}_0) - [E(\lambda\lambda')]K_2'C. \tag{4.29}$$

From Corollary 1.4 of section 3 we have $\text{cov}(\delta_0, \hat{\beta}_0) = 0$. For the second term in (4.29) we calculate

$$\text{cov}(\delta_0, \lambda) = \text{cov}(\delta_0, K_2'\hat{\beta}_0 - m_2)(K_2'CK_2)^{-1} \tag{4.30}$$

$$= \text{cov}(\delta_0, \hat{\beta}_0)K_2(K_2'CK_2)^{-1} = 0.$$

For the third term we calculate

$$\text{cov}(\lambda, \hat{\beta}_0) - [E(\lambda\lambda')]K_2'C \tag{4.31}$$

$$= (K_2'CK_2)^{-1}\,\text{cov}(K_2'\hat{\beta}_0 - m_2, \hat{\beta}_0) - (\text{var}\,\lambda)K_2'C$$

$$= (K_2'CK_2)^{-1}\{K_2'\,\text{var}(\hat{\beta}_0) - K_2'C\sigma^2\}$$

$$= (K_2'CK_2)^{-1}\{K_2'\,\text{var}(CXY) - K_2'C\sigma^2\} = 0.$$

Substituting in (4.29) we obtain the desired result (4.28).

It is possible to develop the extension of the Gauss theorem in a manner which leans more heavily on properties of the weak generalized inverse. However, the final form of the solution is not useful for practical applications. One possible advantage of this alternative approach is that there is no need to make a distinction between pre-estimable and nonpre-estimable functions. These results are contained in the following theorem.

THEOREM 3. *Let* X, β *and* Y *be as before, satisfying*

$$E(Y) = X'\beta,\ \text{var}(Y) = \sigma^2 I$$

and also the restraints

$$L'\beta = m \tag{4.32}$$

where L *is a* $p \times k$ *matrix of known constants and* m *is a* $k \times 1$ *vector of known constants. The minimum variance unbiased linear estimate of any estimable linear function* $\theta = l'\beta$ *is* $\hat{\theta} = l'\hat{\beta}$, *where* $\hat{\beta}$ *(independent of* l*) is given by*

$$\hat{\beta} = (I - LL^-)'\tilde{C}(I - LL^-)XY$$

$$+ [I - (I - LL^-)'\tilde{C}(I - LL^-)A](L^-)'m \tag{4.33}$$

and $\tilde{C}$ *is related to* $\tilde{A} = (I - LL^-)A(I - LL^-)'$ *as* C *is to* A.

PROOF. We first show that the unbiased linear estimates of $\theta = l'\beta$ are precisely the linear forms

$$g(Y) = d'Y + \rho' m \tag{4.34}$$

for which

$$Xd + L\rho = l \tag{4.35}$$

where d is an $n \times 1$ vector and ρ is a $k \times 1$ vector. Thus θ is estimable if and only if (4.35) has a solution (d, ρ). The proof is based on the observation that

$$Z' = [Y', m'] \tag{4.36}$$

defines an $(n+k) \times 1$ random vector Z (recall that a constant is a special case of a random variable), and that (4.32) and $E(Y) = X'\beta$ are equivalent to $E(Z) = [X, L]'\beta$. Thus the assertion is proved by the proof of eq (3.4), with Z replacing Y, $[X, L]$ replacing X, and $[d', \rho']$ replacing d'.

The variance of $g(Y)$ given by (4.34) is $(d'd)\sigma^2$, so that finding a best estimate of θ is equivalent to minimizing $d'd$ by a proper choice of d, subject to the condition that there exist a ρ related to d by (4.35). The choice of such a ρ is immaterial (as long as one exists) since ρ appears in (4.34) only in the combination

$$\rho' m = (L\rho)'\beta$$

which by eq (4.35) is determined by d and l. If d is such that some ρ obeys (4.35), then by eq (2.6a)

$$l - Xd = L\rho = LL^-L\rho = LL^-(l - Xd)$$

with L^- any weak generalized inverse of L, so that

$$(I - LL^-)(l - Xd) = 0 \tag{4.37}$$

and a particular solution of (4.35) is $\rho^* = L^-(l - Xd)$. Conversely if (4.37) is satisfied then ρ^* provides a solution of eq (4.35) and we can take

$$g(Y) = d'(Y - X'(L^-)'m) + l'(L^-)'m. \tag{4.38}$$

It has been shown that finding a best estimate of θ is equivalent to minimizing $d'd$ subject to condition (4.37), which can be rewritten as $\tilde{X}d = \tilde{l}$ with

$$\tilde{X} = (I - LL^-)X,\ \tilde{l} = (I - LL^-)l.$$

[16] If the column vector Z is such that $E(Z) = 0$, $\text{var}\,Z = \sigma^2\Sigma$, then $E(Z'AZ) = \sigma^2\,\text{tr}\,A\Sigma$.

This is analogous to the problem (treated in the proof of the Gauss theorem) of minimizing $d'd$ subject to $Xd=l$, and so the unique solution is

$$\hat{d}=\tilde{X}-\tilde{l}=X'(I-LL^-)'\tilde{C}(I-LL^-)l, \qquad (4.39)$$

from which eq (4.33) follows by substitution into (4.38).

Still another approach to the material of the section can be based on the random variable Z defined by eq (4.36). Namely, as regards the first and second moments with which least-squares theory is exclusively concerned, the model specified by $E(Y)=X'\beta$ and $L'\beta=m$ is equivalent to the model

$$E(Z)=[X, L]'\beta, \text{ var}(Z)=\sigma^2\begin{bmatrix} I_n & 0 \\ 0 & 0_k \end{bmatrix} \qquad (4.40)$$

where I_n is the $n\times n$ identity matrix and 0_k is the $k\times k$ zero matrix. Thus a model with linear restraints is equivalent to a "restraintless" model which however involves a singular variance-covariance matrix. Least-squares estimation in such models is discussed in the next section.

5. Gauss Theorem With Arbitrary Variance-Covariance Matrix

The results of the previous sections were derived assuming that the vector of random variables $Y'=(Y_1, Y_2, \ldots, Y_n)$ were uncorrelated and had common variance; i.e., var $Y=\sigma^2 I$. This section considers some ramifications when var $Y=\sigma^2 V$ where V is a known $n\times n$ matrix with rank m $(m\leq n)$. The case when $m=n$ has been investigated by Aitken [1937]. His result is generalized to include the possibility of a singular variance-covariance matrix.

5.1. Preliminaries

Before discussing the extension of Aitken's results it will be convenient to record the implications of having a singular variance-covariance matrix. When V is singular with rank m $(m<n)$, then there will exist a $n\times s$ $(s=n-m)$ matrix F with rank s such that $F'V=0$. However, this also implies that the s components of $F'Y$ have var $F'Y=(F'VF)\sigma^2=0$ which is equivalent to $F'Y$ being equal to a constant.[17] Since $E(Y)=X'\beta$, we have as the value of this constant

$$F'Y=F'E(Y)=F'X'\beta. \qquad (5.1)$$

Then the distribution of $Y'=(Y_1, Y_2, \ldots, Y_n)$ is singular and can be reduced to a distribution in m random variables. In most applications when (5.1) holds we generally have $F'X'=0$. However, it is quite possible that $F'X'\neq 0$. In order to discuss this more general problem, we write $F=(F_1, F_2)$ in partitioned form where F_i is $n\times s_i$ with rank s_i $(i=1, 2)$ and $s_1+s_2=s$. Furthermore we have

$$F_1'X'=0 \qquad (5.2)$$

$$\text{rank } F_2'X'=s_2 \qquad (s_2<p).$$

[17] The qualifying phrase "with probability one" should be added but we omit such distinctions.

Note that (5.2) combined with (5.1) results in

$$F_1'Y=0 \qquad (5.3)$$

$$F_2'X'\beta=F_2'Y.$$

That is, there are s_1 independent linear relations among $(Y_1, Y_2, \ldots, Y_n)$ and s_2 restraints among the β which are preestimable by virtue of $H'(XF_2)=0$.

Another preliminary aspect of the problem is the existence of an $n\times n$ orthogonal matrix P such that

$$P'VP=\begin{bmatrix} 0 & 0 \\ 0 & \Lambda \end{bmatrix} \qquad (5.4)$$

where Λ is the $m\times m$ diagonal matrix whose elements are the m nonzero characteristic roots of the symmetric positive semidefinite matrix V. Let G be a $n\times m$ matrix such that the columns of G are the m (normalized) characteristic vectors of V; i.e.,

$$VG=G\Lambda, \qquad G'G=I$$

Then the orthogonal matrix P in (5.4) can be taken to be

$$P=[F,G] \qquad (5.5)$$

where F is the $n\times s$ matrix mentioned previously, chosen (as is possible) so that $F'F=I$ and $G'F=0$. By virtue of this partition we have

$$V=G\Lambda G'. \qquad (5.6)$$

We also note that V^+ is given by

$$V^+=G\Lambda^{-1}G'.$$

The necessary four properties (2.1a–d) follow from

$$V^+V=G\Lambda^{-1}G'G\Lambda G'=GG'$$

as $G'G=I$.

A frequently occurring case is when $V^2=cV$ where c is a scalar. Then it can readily be verified that the generalized inverse of V is $V^+=c^{-2}V$.

Also there will be need for writing the matrix V^+ as

$$V^+=TT', \quad T=G\Lambda^{-1/2} \qquad (5.7)$$

where $\Lambda^{-1/2}$ denotes the matrix obtained from Λ by replacing the diagonal terms by the reciprocals of their positive square roots. Note also that $T'VT=I$.

5.2. Arbitrary Variance-Covariance Matrix

In this subsection we give some of the main results associated with an arbitrary variance-covariance matrix. The notation used will correspond to that of the preceding sections.

THEOREM 4. *Consider the vector of random variables* Y *having* $E(Y)=X'\beta$, var $(Y)=\sigma^2 V$ *where* V *is an* $n\times n$ *symmetric positive semidefinite matrix with rank* m $(m\leq n)$. *Then the minimum variance linear unbiased estimate of* $\theta=l'\beta$ *coincides with its best*

estimate found from the model

$$E(\tilde{Y}) = \tilde{X}'\beta, \text{ var } \tilde{Y} = \sigma^2 I. \tag{5.8}$$

$$\tilde{K}'\beta = \tilde{m}$$

where $\tilde{X} = XT$, $\tilde{Y} = T'Y$, $\tilde{K} = XF_2$ *and* $\tilde{m} = F_2'Y$. *Thus if* F_2 *is null,* $\hat{\beta}$ *can be chosen as any solution of the normal equations*

$$(XV^+X')\hat{\beta} = XV^+Y. \tag{5.9}$$

PROOF. As in the proof of the Gauss theorem of section 3, obtaining a best estimate $\Delta'Y + c$ of θ is equivalent to choosing an $n \times 1$ vector Δ, subject to $X\Delta = l$, so as to minimize

$$\text{var}(\Delta'Y) = (\Delta'V\Delta)\sigma^2.$$

On the other hand, from the beginning of the proof of Theorem 3 we see that finding a best estimate in the model (5.8) is equivalent to choosing a pair $[d', \rho']$, where d is an $m \times 1$ vector and ρ an $s_2 \times 1$ vector, so as to minimize $d'd$ subject to

$$\tilde{X}d + \tilde{K}\rho = l,$$

i.e.,
$$X(Td + F_2\rho) = l.$$

Thus the theorem will be proved if we show how to associate to each vector Δ a pair $[d', \rho']$, and to each pair $[d', \rho']$ a vector Δ, such that in each case

$$X\Delta = X(Td + F_2\rho),\ \Delta'V\Delta = d'd. \tag{*}$$

Given $[d', \rho']$ we simply set $\Delta = Td + F_2\rho$; the second relation in (*) then follows from $F'V = 0$ and $T'VT = I$. Given Δ, we employ the orthogonal matrix

$$P = [F, G] = [F_1, F_2, G]$$

to define an $n \times 1$ vector (and thus define d and ρ) by

$$[\rho_1', \rho', d'\Lambda^{-1/2}]' = P^{-1}\Delta;$$

then we have

$$\Delta = P[\rho_1', \rho', d'\Lambda^{-1/2}]' = F_1\rho_1 + F_2\rho + Td$$

The first requirement of (*) is satisfied because $XF_1 = 0$, and the second for the same reasons as above.

Finally, that the normal equations corresponding to the first line of (5.8) are given by (5.9) follows from substitution for the tilde quantities, together with $TT' = V^+$.

COROLLARY 4.1 (Aitken). *If* V *is non-singular then the best estimate of any estimable* $\theta = l'\beta$ *is given by* $\hat{\theta} = l'\hat{\beta}$ *where* $\hat{\beta}$ *is any solution of the normal equations*

$$(XV^{-1}X')\hat{\beta} = XV^{-1}Y. \tag{5.10}$$

PROOF. When V is nonsingular, the matrix F is null and $V^+ = V^{-1}$, so the result follows from (5.9).

COROLLARY 4.2. *Let* $\tilde{X} = XT$ *have rank* q. *Then the minimum variance linear unbiased estimate of an estimable function is* $\hat{\theta} = l'\hat{\beta}$ *where*

$$\hat{\beta} = \tilde{C}XV^+Y + \tilde{C}\tilde{K}(\tilde{K}'\tilde{C}\tilde{K})^{-1}(\tilde{m} - \tilde{K}'\tilde{C}XV^+Y) + H(K'H)^{-1}m_0.$$

The matrix $\tilde{C}$ *is related to* $\tilde{A} = \tilde{X}\tilde{X}' = XV^+X'$ *and* $\tilde{K}$ *by* Lemmas 1 *and* 2; $\tilde{K}$ *is a* $p \times r$ $(r = p - q)$ *matrix of rank* r *such that* $\det H'K \neq 0$, *and* m_0 *is an arbitrary* $r \times 1$ *vector.*

PROOF. Since $\tilde{X} = XT$ has rank q, H has the same relation to $\tilde{X}$ as to X. Because $H'\tilde{K} = 0$, the restraints $\tilde{K}'\beta = \tilde{m}$ are pre-estimable in the model (5.8). The result follows from (4.15) upon noting that here H_1 and K_1 are null, while $H_0 = H$ and $K_0 = \tilde{K}$.

COROLLARY 4.3. *If* $\tilde{X}$ *has rank* q, *then the quantity*

$$S^2 = (\tilde{Y} - \tilde{X}'\tilde{\beta}_0)'(\tilde{Y} - \tilde{X}'\tilde{\beta}_0) + \tilde{\lambda}'(\tilde{K}'\tilde{C}\tilde{K})\tilde{\lambda},$$

in which

$$\tilde{\beta}_0 = \tilde{C}\tilde{X}\tilde{Y} = \tilde{C}XV^+Y$$

$$\tilde{\lambda} = (\tilde{K}'\tilde{C}\tilde{K})^{-1}(\tilde{K}'\tilde{C}\tilde{X}\tilde{Y} - \tilde{m}),$$

has expectation

$$E(S^2) = (m - q + s_2)\sigma^2.$$

PROOF. This corollary is an application of corollary 2.4 of section 4 to the model (5.8). Note that $\tilde{X}$ is $p \times m$, which is why m appears in place of n in the formula for $E(S^2)$.

The first two sentences of the proof of corollary 4.2 show that if $\tilde{X} = XT$ has rank q, then the class of pre-estimable functions is not reduced in passing to the model (5.8). However if $\tilde{X}$ has rank $\tilde{q}(\tilde{q} < q)$, then in passing to (5.8) H is replaced by a $p \times \tilde{r}$ matrix $\tilde{H}$ of rank $\tilde{r} = p - \tilde{q}$ such that $\tilde{H}'X = 0$. Such a matrix can be obtained as $\tilde{H} = [H_0, H]$ where H_0 is an appropriate $p \times (q - \tilde{q})$ matrix.

It is desirable to have a system of equations for $\hat{\beta}$ (in Theorem 4) when F_2 is *not* null. Such systems can be obtained (and other information derived) by applying the material of section 4 to the model (5.8). In doing so it should be kept in mind that the restraints $\tilde{K}'\hat{\beta} = \tilde{m}$ must be separated into those which are pre-estimable (this is the sole class when $\tilde{q} = q$, as already noted), and those which are not; the latter must be examined for irreducibility (see the paragraph preceding Theorem 2) and "reduced" if necessary.

It is natural, as a next step, to consider a model which involves *both* the complications of linear restraints on the β and an arbitrary variance-covariance matrix $V\sigma^2$. This requires no new extension of the

theory, since the only addition is that of the restraints $K_i'\beta = m_i$ $(i=1, 2)$ where $K_2'\beta$ represent pre-estimable restraints. It is quite possible that some of the restraints $K'\beta$ coincide with the restraints $\bar{K}'\beta$ in which case the duplicate restraints in $K_2'\beta$ (or $\bar{K}_2'\beta$) may be dropped. Aside from this duplication one will then have the situation

$$E(Y)=X'\beta,\ \text{var}\ Y=\sigma^2V\ (V\ \text{has rank}\ m\ (m\leqslant n))$$

$$K_i'\beta=m_i\ (i=1, 2)$$

which is identical for purposes of estimating $\theta=l'\beta$ with

$$\begin{aligned} &E(\tilde{Y})=\tilde{X}'\beta,\ \text{var}\ \tilde{Y}=\sigma^2I \\ &K_i'\beta=m_i,\ \bar{K}'\beta=\bar{m} \end{aligned} \tag{5.11}$$

where the tilde ($\tilde{}$) quantities are defined as in Theorem 4. A formal proof is obtained by applying Theorem 4 to

$$E(Y^*)=(X^*)'\beta,\ \text{var}\ Y^*=V^*\sigma^2$$

in which

$$(Y^*)'=[Y',\ m_1',\ m_2'],\ X^*=[X,\ K_1,\ K_2],$$

$$V^*=\begin{bmatrix} V & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Suppose for example that X is of full rank (i.e., $q=p$) and that V is nonsingular (i.e., $m=n$), and consider the model [17a]

$$E(Y)=X'\beta,\ \text{var}(Y)=\sigma^2V \tag{5.11a}$$

$$K'\beta=m,$$

where K is a $p\times k$ matrix of rank k and m is a $k\times 1$ vector, both consisting of known constants. By the prescription given in the last paragraph, and from the fact that $m=n$ implies that $\bar{K}$ in Theorem 4 is null, we see that an appropriate $\tilde{\beta}$ will be one for the model

$$E(\bar{Y})=\bar{X}'\beta,\ \text{var}\ (\bar{Y})=\sigma^2I \tag{5.11b}$$

$$K'\beta=m \tag{5.11c}$$

where $\bar{X}=XT$, $\bar{Y}=T'Y$, and $T=G\Lambda^{-1/2}$. G is of rank $m=n$ and so T is $n\times n$ nonsingular, implying (since $q=p$) that $\bar{X}$ is of rank p. Hence the constraints $K'\beta$ are all pre-estimable with respect to (5.11b), i.e. $K=K_2$ in our previous notation. Applying (4.20), we see that we can take

$$\hat{\beta}=\tilde{\beta}_0+\tilde{C}K(K'\tilde{C}K)^{-1}(m-K'\tilde{C}\tilde{X}\tilde{Y}) \tag{5.11d}$$

[17a] In the rest of this subsection, use of the symbol m both for the rank of V (here $m=n$), and for the $k\times 1$ vector in (5.11a), should cause no confusion.

where $\tilde{C}$ is related to $\tilde{A}=\tilde{X}\tilde{X}'=XV^{-1}X'$ as C is to A, and where $\tilde{\beta}_0$ is the unique solution of $\tilde{A}\tilde{\beta}_0=\tilde{X}\tilde{Y}$. Since $\tilde{A}$ is $p\times p$ nonsingular, we have

$$\tilde{C}=\tilde{A}^{-1}=(XV^{-1}X')^{-1},$$

$$\tilde{\beta}_0=\tilde{C}\tilde{X}\tilde{Y}=(XV^{-1}X')^{-1}XV^{-1}Y,$$

so that substitution in (5.11d) yields

$$\hat{\beta}=(XV^{-1}X')^{-1}\{XV^{-1}Y + K[K'(XV^{-1}X')^{-1}K]^{-1}(m-K'(XV^{-1}X')^{-1}XV^{-1}Y)\},$$

in agreement with the result obtained for this special case by Chipman and Rao [1964].

5.3. Simplification of the Normal Equations

In the model

$$E(Y)=X'\beta,\qquad \text{var}\ Y=\sigma^2V,$$

we will have $XF=0$ (so that the normal equations are given by (5.9)) if and only if $X=XGG'$. For, if this condition holds then

$$XF=(XG)(G'F)=0,$$

while if $XF=0$ then $X=MG'$ for some $p\times m$ matrix M (i.e., the rows of X are linear combinations of the orthonormalized characteristic vectors of V), and postmultiplication by G yields $M=XG$.

In particular, this will be the case if

$$XV^+=BX,\qquad X=BXV \tag{5.12}$$

for some nonsingular $p\times p$ matrix B. For, the first condition in (5.12) yields $X=MG'$ with $M=B^{-1}XG\Lambda^{-1}$, while the second yields it with $M=BXG\Lambda$. The two conditions of (5.12) are logically equivalent, for the first implies

$$X=XGG'=(XG\Lambda^{-1}G')(G\Lambda G')=(XV^+)V=BXV$$

while the second implies

$$XV^+=BXVV^+=BXGG'=BX.$$

If (5.12) holds then the normal equations are

$$(XV^+X')\hat{\beta}=XV^+Y,$$

and become

$$(BXX')\hat{\beta}=BXY,$$

which are equivalent to the usual normal equations $A\hat{\beta}=XY$ obtained when $V=I$. This result seems to have been first noted by T. W. Anderson [1948], and Muller and Watson [1959] have discussed it in the context of randomization theory.

For the rest of this section we assume $XF=0$ (i.e., $X=XGG'$), and ask when a simplification of the normal equations something like the one described above is possible. Note that $X=XGG'$ implies $q \leqslant m$. If $q=m$ we can partition

$$X'=[X_1', X_2'], \quad \beta'=[\beta_1', \beta_2']$$

where X_1 is $q\times n$ of rank q, X_2 is $r\times n$, β_1 is $q\times 1$ and β_2 is $r\times 1$. The normal equations become

$$(X_1V^+X_1')\hat{\beta}_1+(X_1V^+X_2')\hat{\beta}_2=X_1V^+Y,$$

$$(X_2V^+X_1')\hat{\beta}_1+(X_2V^+X_2')\hat{\beta}_2=X_2V^+Y.$$

Since $X=XGG'$ implies $X_1=X_1GG'$, X_1G has rank $q=m$ and hence

$$X_1V^+=X_1G\Lambda^{-1}G'=B_1X_1, \qquad B_1=(X_1G)\Lambda^{-1}(X_1G)^{-1}$$

where B_1 is $q\times q$ nonsingular. Premultiplication of the first normal equations by B_1^{-1} (after substitution of B_1X_1 for X_1V^+) yields

$$(X_1X_1')\hat{\beta}_1+(X_1X_2')\hat{\beta}_2=X_1Y \tag{5.13}$$

$$(X_2X_1'B_1')\hat{\beta}_1+(X_2V^+X_2')\hat{\beta}_2=X_2V^+Y.$$

Thus at least the first subsystem of the normal equations has been somewhat simplified.

If in particular $p=q=m$ then we have (5.12) and the resulting full simplification. If $p>q=m$ but $X_1X_2'=0$, then the normal equations reduce to

$$(X_1X_1')\hat{\beta}_1=X_1Y \tag{5.14}$$

$$(X_2V^+X_2')\hat{\beta}_2=X_2V^+Y,$$

and the solutions for $\hat{\beta}_1$ are the same as if var $Y=\sigma^2I$. Without assuming $X_1'X_2=0$, we can observe that $X_2'=X_1'N$ for some $q\times r$ matrix N and that $A_1=X_1X_1'$ is $q\times q$ nonsingular; thus the first subsystem of (5.13) can be solved for $\hat{\beta}_1$ as

$$\hat{\beta}_1=A_1^{-1}X_1Y-N\hat{\beta}_2,$$

and the second subsystem becomes

$$N'(B_1-A_1B_1'A_1^{-1})A_1N\hat{\beta}_2=N'(B_1-A_1B_1'A_1^{-1})X_1Y$$

which is to be solved for $\hat{\beta}_2$. If in addition X_2 has rank r (which requires $r \leqslant g$), then N does too and one can first find the unique $\tilde{\beta}_1$ such that $A_1\tilde{\beta}_1=X_1Y$, and then satisfy the second subsystem by solving $N\hat{\beta}_2=\tilde{\beta}_1$, i.e. $\hat{\beta}_2=(N'N)^{-1}N'\tilde{\beta}_1$.

If $q<m$ the situation is more complicated. This is illustrated by the following example (due to K. Goldberg, NBS) in which $p=q=1$ and $n=m=2$. Take $X=[1, 0]$ and

$$G=G'=2^{-1/2}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}, \qquad \Lambda=\begin{bmatrix}1 & 0\\ 0 & \frac{1}{2}\end{bmatrix}$$

Then $XV^+=XG\Lambda^{-1}G'=[3/2, -1/2]$ but BX has the form $[t, 0]$ for all 1×1 matrices B; hence (5.12) or its analog $X_1V^+=B_1X_1$ cannot hold.

Even when $q<m$, some simplification is possible if there is a partition $G=[G_1, G_2]$, with G_1 ($n\times q$, such that $X_1G_2=0$. For then, if

$$\Lambda=\operatorname{diag}(\Lambda_1, \Lambda_2)$$

denotes the decomposition of Λ corresponding to the partition of G, we have

$$X_1=X_1GG'=X_1(G_1G_1'+G_2G_2')=X_1G_1G_1',$$

$$X_1V^+=X_1(G_1\Lambda_1^{-1}G_1'+G_2\Lambda_2^{-1}G_2')=X_1G_1\Lambda_1^{-1}G_1'$$

and can mimic the procedure for $q=m$ (up to and including (5.14)) using G_1 and Λ_1 instead of G and Λ. At present it is not clear what other cases admit analogous simplification if $q<m$. One such situation arises if we change the dimensions of the partition of X' so that X_i is $p_i\times n$ ($p_1+p_2=p$), β_i is $p_i\times 1$, and X_1 has rank p_1 (implying $p_1 \leqslant q$). If there is a partition $G=[G_1, G_2]$, with G_1 ($p_1\times n$), such that $X_1G_2=0$, then the preceding analysis still applies.

5.4. Equicorrelated Variables

In many experimental situations the covariances between the observations are not zero, but to a reasonable degree of approximation may be regarded as being equal; i.e., cov $(Y_i, Y_j)=\rho\sigma^2$ $(i\neq j)$. Therefore we can write var $Y=V\sigma^2$ where

$$V=(1-\rho)I+\rho J \tag{5.15}$$

and J is an $n\times n$ matrix with all elements unity.

The matrix V has the two distinct characteristic roots $[1+(n-1)\rho]$ and $(1-\rho)$ with multiplicities one and $(n-1)$ respectively. However since $V\sigma^2$ is a variance-covariance matrix, it is positive semidefinite and the roots are nonnegative. Consequently

$$1+(n-1)\rho \geqslant 0, \qquad 1-\rho \geqslant 0$$

and we obtain the bounds $-(n-1)^{-1} \leqslant \rho \leqslant 1$. When either $\rho=-(n-1)^{-1}$ or $\rho=1$, a characteristic root will be zero and V will be singular. If the Y_i are increasing linear functions of one another, ρ will be equal to unity. The case $\rho=-(n-1)^{-1}$ implies that $\sum_{i=1}^{n} Y_i=$ constant, $V^+=(n-1)n^{-1}\{I-J/n\}$, and that the sum of the elements in any row or column of V is zero.

When $\rho\neq 1$ or $\rho\neq(n-1)^{-1}$, V has an inverse which is given by

$$V^{-1}=(1-\rho)^{-1}\{I-\rho[1+(n-1)\rho]^{-1}J\}.$$

Therefore using (5.10) the normal equations can be written

$$\{[A-\rho[1+(n-1)\rho]^{-1}XJX'\}\hat{\beta}=XY-\rho[1+(n-1)\rho]^{-1}XJY. \tag{5.16}$$

where $A=XX'$. The conditions for estimability of a parametric function only involve first moments and hence are not dependent on ρ. Therefore the function $\theta=l'\beta$ is estimable if and only if $H'l=0$ where $H'X=0$. The solution of (5.16) involves knowledge of ρ. However we wish to determine the parametric functions which can be estimated *without* knowledge of ρ.

Let $\mathbf{1}$ denote an $n\times 1$ vector of ones, so that $J=\mathbf{1}\,\mathbf{1}'$. Since $\mathbf{1}$ and therefore $n^{-1/2}\mathbf{1}$ is a characteristic vector of V corresponding to the characteristic root $[1+(n-1)\rho]$, we can take the matrix G of subsection 5.1 as $G=[n^{-1/2}\mathbf{1}, M]$. Here the $n-1$ columns of M are characteristic vectors of V corresponding to the characteristic root $(1-\rho)$, and

$$M'M=I_{n-1}, \qquad \mathbf{1}'M=0, \qquad VM=(1-\rho)M.$$

Since G is square, $G'G=I$ implies $GG'=I$ and therefore

$$MM'=I-n^{-1}J.$$

Also, in the notation of subsection 5.1,

$$T=G\Lambda^{-1/2}=[n^{-1/2}(1+(n-1)\rho)^{-1/2}\mathbf{1}, (1-\rho)^{-1/2}M],$$

so in applying Theorem 4

$$\tilde{X}=XT=[n^{-1/2}(1+(n-1)\rho)^{-1/2}X\mathbf{1}, (1-\rho)^{-1/2}XM],$$

$$\tilde{Y}=T'Y=\begin{bmatrix} n^{-1/2}(1+(n-1)\rho)^{-1/2}\mathbf{1}'Y \\ (1-\rho)^{-1/2}M'Y \end{bmatrix}.$$

The equation $E(\tilde{Y})=\tilde{X}'\beta$ of (5.8) therefore becomes equivalent to

$$E(\mathbf{1}'Y)=\mathbf{1}'X'\beta, \tag{5.17}$$

$$E(\overline{Y})=\overline{X}'\beta \qquad (\overline{X}=XM, \overline{Y}=M'Y) \tag{5.18}$$

and it is readily verified that

$$\operatorname{var}(\overline{Y})=(1-\rho)\sigma^2 I, \qquad \operatorname{cov}(\mathbf{1}'Y, \overline{Y})=0. \tag{5.19}$$

The unbiased estimates of any estimable $\theta=l'\beta$ have the form

$$g(Y)=d'\overline{Y}+e(\mathbf{1}'Y)$$

where d is an $(n-1)\times 1$ vector, e is a scalar, and

$$\overline{X}d+X\mathbf{1}e=l. \tag{5.20}$$

Also,

$$\operatorname{var}[g(Y)]=(1-\rho)\sigma^2 d'd+e^2 n[1+(n-1)\rho]\sigma^2$$
$$=(1-\rho)\sigma^2[d'd+e^2 n]+e^2 n^2\rho\sigma^2.$$

First suppose the rank of $\overline{X}=XM$ is less than the rank q of X. This rank must be $q-1$. Then there exists an $m\times 1$ vector h such that $h'X=\mathbf{1}$, and (5.20) yields

$$h'l=h'XMd+h'X\mathbf{1}e=ne,$$

so that

$$e=e_0=n^{-1}(l'h)$$

in every estimate $g(Y)$.[18] Thus the minimization of $\operatorname{var}[g(Y)]$ subject to (5.20) is achieved by choosing d to minimize $d'd$ subject to

$$Xd=l-X\mathbf{1}e_0=l-Ahe_0.$$

This, however, coincides with the problem of finding a best estimate for $(l-Ahe_0)'\beta$ in the model specified by (5.18) and (5.19); the Gauss theorem yields the solution as

$$d'\overline{Y}=(l-Ahe_0)'\tilde{\beta}$$

where $\tilde{\beta}$ is any solution of the normal equations obtained using (5.18) and (5.19). Since $MM'=I-n^{-1}J$, we find that these normal equations are

$$X[I-n^{-1}J]X'\tilde{\beta}=X[I-n^{-1}J]Y. \tag{5.21}$$

Thus the best estimate $g(Y)$ of $\theta=l'\beta$ is

$$\begin{aligned}\hat{\theta}&=(l-Ahe_0)'\tilde{\beta}+\mathbf{1}'Ye_0\\ &=l'\tilde{\beta}-l'h(n^{-1}h'A\tilde{\beta})+l'h(n^{-1}\mathbf{1}'Y)\\ &=l'\hat{\beta}\end{aligned}$$

where $\hat{\beta}=\tilde{\beta}+n^{-1}h(\mathbf{1}'Y-\mathbf{1}'X'\tilde{\beta})$. Use of (5.21) and $h'X=\mathbf{1}'$ leads to $A\hat{\beta}=XY$. Conversely if $\hat{\beta}$ is any solution of $A\beta=XY$, then choosing $\tilde{\beta}=\hat{\beta}$ yields a solution of (5.21), and also

$$\hat{\theta}=(l-Ahe_0)'\hat{\beta}+\mathbf{1}'Ye_0=l'\hat{\beta}.$$

Now assume $\overline{X}=XM$ has the same rank q as X. To minimize $\operatorname{var}[g(Y)]$, first treat e as fixed; as in the previous case we are led to the choice

$$d'\overline{Y}=(l-X\mathbf{1}e)'\tilde{\beta}$$

where $\tilde{\beta}$ is any solution of (5.21). The rank hypothesis implies that the same H, and thus the same K and C, work for $\overline{X}\overline{X}'$ as for A, and so we may choose $\tilde{\beta}=C\overline{X}\overline{Y}$. Now

$$g(Y)=l'\tilde{\beta}+e\mathbf{1}'(Y-X'\tilde{\beta})$$

$$\operatorname{var}[g(Y)]=\operatorname{var}(l'\tilde{\beta})+e^2\operatorname{var}[\mathbf{1}'(Y-X'\tilde{\beta})]$$
$$+2e\operatorname{cov}[l'\tilde{\beta}, \mathbf{1}'(Y-X'\tilde{\beta})].$$

The range of e in the remaining minimization problem is that of all real numbers. To prove this, note that by the rank hypothesis $l=\overline{X}d_0$ for some $(n-1)\times 1$

[18] A simple sufficient condition for the existence of such a vector h is that the columns of X all sum to some nonzero constant k. That is, $\mathbf{1}'X=k\mathbf{1}'$ and thus we may take $h=k^{-1}\mathbf{1}$.

vector d_0 (i.e., each estimable form is also estimable with respect to (5.18)), and also $X = \bar{X}N$ for some matrix N, so that for any real number e

$$l - X\mathbf{1}e = \bar{X}d \qquad (d = d_0 - N\mathbf{1}e)$$

as required by (5.20). The solution of the minimization problem is therefore

$$e = -\operatorname{cov}[l'\tilde{\beta},\ \mathbf{1}'(Y - X'\tilde{\beta})]/\operatorname{var}[1'(Y - X'\tilde{\beta})]$$

$$= (1-\rho)l'CX\mathbf{1}/\{n[1+(n-1)\rho] + (1-\rho)\mathbf{1}'X'CX\mathbf{1}\}.$$

This is independent of ρ if and only if the numerator vanishes, i.e.,

$$l'CX\mathbf{1} = 0, \tag{5.22}$$

and in that event the best estimate reduces to

$$l'\tilde{\beta} = l'CX(I - n^{-1}J)Y = l'CXY = l'\hat{\beta}$$

where $\hat{\beta}$ is a solution of $A\hat{\beta} = XY$. Note that $l'CX\mathbf{1} = 0$ will hold for *all* estimable functions if and only if $X\mathbf{1} = 0$.

Before assembling these results (with a few more substitutions) into a formal theorem, we remark that XM has the same rank as

$$XMM'X' = X(I - n^{-1}J)X' = X(I - n^{-1}J)^2X',$$

and thus the same rank as the matrix

$$X^* = X[I - n^{-1}J]$$

obtained from X by simply taking deviations from the mean, i.e.,

$$x^*_{i\alpha} = x_{i\alpha} - \bar{x}_i; \qquad \bar{x}_i = n^{-1}\sum_{\alpha=1}^{n} x_{i\alpha}.$$

Thus when X^* and X have the same rank, a solution of (5.21) can be obtained as

$$\tilde{\beta} = CX[I - n^{-1}J]Y = \hat{\beta} - n^{-1}CXJY.$$

THEOREM 5. *Let*

$$\mathrm{E}(\mathrm{Y}) = \mathrm{X}'\beta,\ \operatorname{var}(\mathrm{Y}) = \sigma^2[(1-\rho)\mathrm{I} + \rho\mathrm{J}],$$

$-(n-1)^{-1} < \rho < 1$. *If the rank* q^* *of* $X^* = X[I - n^{-1}J]$ *is* $q-1$ (*i.e., there exists an* $n\times 1$ *vector* h *such that* $h'X = \mathbf{1}'$), *the normal equations are* $A\hat{\beta} = XY$ *and do not depend on* ρ. *When* $q^* = q$, *the only estimable functions* $\theta = l'\beta$ *with best estimate independent of* ρ *are those with*

$$l'CX\mathbf{1} = 0, \tag{5.22}$$

and for these the best estimate is $l'\hat{\beta}$ *with* $A\hat{\beta} = XY$. *If* (5.22) *does not hold, the best estimate of* θ *is*

$$\hat{\theta} = l'[\hat{\beta} - n^{-1}CXJY + \{n[n\rho(1-\rho)^{-1} + 1] + \mathbf{1}'X'CX\mathbf{1}\}^{-1}$$

$$(Y - X'\hat{\beta} + n^{-1}X'CXJY)]$$

with $\hat{\beta}$ *as above.*

COROLLARY 5.1. *Let the deviations* Y^* *and* X^* *be defined by* $Y^* = M\bar{Y} = MM'Y$, $X^* = \bar{X}M' = XMM'$. *Then the quantity*

$$S^2 = (Y^* - X^{*\prime}\hat{\beta})'(Y^* - X^{*\prime}\hat{\beta})$$

has expectation

$$\mathrm{E}(S^2) = (n-q)(1-\rho)\sigma^2$$

if a vector h *exists for which* $h'X = \mathbf{1}'$; *otherwise the expectation of* S^2 *is*

$$\mathrm{E}(S^2) = (n-q-1)(1-\rho)\sigma^2.$$

PROOF. The expectation of $(\bar{Y} - \bar{X}'\hat{\beta})'(\bar{Y} - \bar{X}'\hat{\beta})$ is $(n-q)(1-\rho)\sigma^2$ if $\bar{X}$ has rank $q-1$ (i.e., a vector h exists for which $h'X = 1$). When X has rank q, the expectation is $(n-q-1)(1-\rho)\sigma^2$. These results immediately follow by applying corollary 1.4 of the Gauss theorem. Since

$$\bar{Y} - \bar{X}'\hat{\beta} = M'(Y - X'\hat{\beta})$$

and $(MM')^2 = MM' = I - n^{-1}J$, we have

$$(\bar{Y} - \bar{X}'\hat{\beta})'(\bar{Y} - \bar{X}'\hat{\beta}) = (Y - X'\hat{\beta})'MM'(Y - X'\hat{\beta})$$
$$= (Y^* - X^{*\prime}\beta)'(Y^* - X^{*\prime}\hat{\beta}).$$

The problem arises as to what to do if there does not exist an h for which $h'X = \mathbf{1}'$ (i.e., if XM has the same rank q as X), ρ is unknown, and we wish to estimate an estimable function for which $l'CX\mathbf{1} \neq 0$. Estimates of $\theta = l'\beta$ can be obtained *if* we are willing to consider the alternate estimation problem where

$$E(\bar{Y}) = \bar{X}'\beta,\ \operatorname{var}\bar{Y} = (1-\rho)\sigma^2 I \tag{5.23}$$

subject to the restraint

$$\mathbf{1}'X'\beta = \mathbf{1}'Y,$$

which must be pre-estimable.

Application of (4.16) results in the normal equations

$$X(I - n^{-1}J)X'\hat{\beta} + X\mathbf{1}\lambda = X(I - n^{-1}J)Y,$$

$$\mathbf{1}'X'\hat{\beta} = \mathbf{1}'Y,$$

which reduce to

$$A\hat{\beta} + X\mathbf{1}\lambda = XY,$$

$$\mathbf{1}'X'\hat{\beta} = \mathbf{1}'Y.$$

After premultiplication by the nonzero $1\times p$ vector $\mathbf{1}'X'$, the first equation can be solved for λ to obtain

$$\lambda=(\mathbf{1}'X'X\mathbf{1})^{-1}\mathbf{1}'X'(XY-A\hat{\beta}),$$

and then the normal equations for $\hat{\beta}$ alone are obtained as

$$[I-(\mathbf{1}'X'X\mathbf{1})^{-1}XJX']A\hat{\beta}=[I-(\mathbf{1}X'X\mathbf{1})^{-1}XJX']XY$$

$$\mathbf{1}'X'\hat{\beta}=\mathbf{1}'Y.$$

Alternatively, we can apply Theorem 2 to the model given by (5.23) and the restraint $\mathbf{1}'X'\beta=\mathbf{1}'Y$. Since $\overline{X}$ has the same rank as X, H has the same relation to $\overline{X}$ as to X. Thus, by Lemmas 1 and 2, the matrices K and C are the same for $\overline{X}$ as for X. Here H_1 and K_1 are null, while H_0 and K_0 correspond to H and K, respectively. The result of applying Theorem 2 is given next as another theorem; note that the estimate $\hat{\theta}=l'\hat{\beta}$ coincides with that given in Theorem 5 when $l'CX\mathbf{1}=0$.

THEOREM 6. *For the model*

$$\mathrm{E(Y)=X'\beta,}\qquad \mathrm{var\ Y=\sigma^2[(1-\rho)I+\rho J],}$$

where $-(n-1)^{-1}<\rho<1$, *the parameter* ρ *is unknown, and* $\overline{X}=XM$ *has the same rank as* X, *the best estimate conditional on* $\mathbf{1}'X'\beta=\mathbf{1}'Y$ *of the estimable function* $\theta=l'\beta$ *is given by*

$$\hat{\theta}=l'\hat{\beta}=l'CX\{(I-n^{-1}J)$$

$$+(\mathbf{1}'X'CX\mathbf{1})^{-1}J[I-X'CX(I-n^{-1}J)]\}Y. \quad (5.24)$$

COROLLARY 6.1. *The quantity*

$$S^2=(Y^*-(X^*)'\hat{\beta})'(Y^*-(X^*)'\hat{\beta}),$$

where $X^*=X(I-n^{-1}J)$ *and* $Y^*=(I-n^{-1}J)Y$, *has the conditional expectation*

$$E(S^2|\mathbf{1}'Y)=(1-\rho)\sigma^2(n-q).$$

PROOF. We first observe that

$$S^2=(\overline{Y}-\overline{X}'\hat{\beta})'(\overline{Y}-\overline{X}'\hat{\beta}),$$

so that $E(S^2|\mathbf{1}'Y)$ can be found by applying Corollary 2.4 to the model consisting of (5.23) and the restraint $\mathbf{1}'X'\beta=\mathbf{1}'Y$. Here $k_2=1$, n is replaced by $n-1$ since $\overline{X}$ is $p\times(n-1)$, and σ^2 is replaced by $(1-\rho)\sigma^2$. This proof also shows, by (4.27), that S^2 can be written as

$$S^2=(Y^*-(X^*)'\hat{\beta}_0)'(Y^*-(X^*)\hat{\beta}_0)+\lambda^2(\mathbf{1}'X'CX\mathbf{1})$$

where $\hat{\beta}_0=CX(I-n^{-1}J)Y$ and

$$\lambda=(\mathbf{1}'X'CX\mathbf{1})^{-1}[\mathbf{1}'X'CX(I-n^{-1}J)Y-\mathbf{1}'Y].$$

5.5. Two Stage Least Squares

An application of Theorem 4 arises in two stage least squares estimation which has recently been discussed by Freund, Vail, and Clunies-Ross (1961) and Goldberger and Jockems (1961). We shall consider some further generalizations and discuss the matter more fully. Consider the model

$$E(Y)=X_1'\beta_1+X_2'\beta_2,\ \mathrm{var}\ Y=\sigma^2I \quad (5.25)$$

where X_i are $p_i\times n$ matrices and β_i are $p_i\times 1$ vectors for $i=1, 2$. Instead of considering the full model, in the first stage we ignore β_2 variables and take $E(Y)=X_1'\beta_1$. Then the normal equations will yield the solution

$$\tilde{\beta}_1=C_1X_1Y \quad (5.26)$$

where C_1 is related to X_1X_1' as C is to A.

Define the residual vector

$$\delta=Y-X_1'\tilde{\beta}_1=(I-X_1'C_1X_1)Y$$

and the idempotent matrix

$$V=I-X_1'C_1X_1.$$

Then we have

$$E(\delta)=VX_2'\beta_2,$$

$$\mathrm{var}\,(\delta)=V\sigma^2,$$

and these equations serve as the model for the *second* stage. Now apply Theorem 4 to this model: $V=V^+$ since V is idempotent, the analogs of X and $F'=F_1'$ are X_2V and X_1 respectively with $X_1(X_2V)'=0$ since $X_1V=0$, and so the result is the equation

$$(X_2VX_2')\hat{\beta}_2=X_2V\delta=X_2VY \quad (5.27)$$

with solution

$$\hat{\beta}_2=C_2X_2V\delta=C_2X_2VY, \quad (5.28)$$

where C_2 is related to X_2VX_2' as is C to A.

Suppose $\theta=l_1'\beta_1+l_2'\beta_2$ is estimable in the full model. Then (see (3.4)) there exists an $n\times 1$ vector d such that $X_id=l_i(i=1, 2)$, and so $\theta_1=l_1'\beta_1$ is estimable in the first-stage model. Its best estimate in that model is

$$\tilde{\theta}_1=l_1'\tilde{\beta}_1,$$

and in the full model

$$E(\tilde{\theta}_1)=l_1'C_1X_1(X_1'\beta_1+X_2'\beta_2)=\theta_1+l_1'C_1X_1X_2'\beta_2. \quad (5.29)$$

The procedure to be described involves adding a term to $\tilde{\theta}_1$ to obtain an unbiased estimate $\hat{\theta}_1$ of θ_1. Clearly this will be possible only if θ_1 is in fact estimable in the full model. We therefore are led to determine what condition on the partition $[X_1', X_2']$ will ensure that $\theta_1=l_1'\beta_1$ is estimable in the full model whenever $\theta=l'\beta$ is. First suppose the partition has this property. Since the rows of $X'\beta$ are estimable in the full model, the same must hold for the rows of $X_1'\beta_1$ and thus for the rows of

$$X_2'\beta_2=X'\beta-X_1'\beta_1.$$

By (3.4) there is an $n\times n$ matrix B such that $X_1B=0$ and $X_2B=X_2$. $X_1B=0$ implies that $B=VB_1$ for some $p_1\times n$ matrix B_1, and so $X_2VB_1=X_2$. The last equation shows that the rows of $X_2'\beta_2$ are estimable in the second-stage model, or equivalently (by Corollary 1.1)

$$X_2=X_2VX_2'C_2X_2. \tag{5.30}$$

Conversely, suppose (5.30) holds and that

$$\theta=l_1'\beta_1+l_2'\beta_2$$

is any parametric function estimable in the full model. By (3.4), there exists an $n\times 1$ vector d such that

$$X_id=l_i\ (i=1,2).$$

Then

$$X_1(I-VX_2'C_2X_2)d=l_1,\ X_2(I-VX_2'C_2X_2)d=0$$

so that by (3.4) $\theta_1=l_1'\beta_1$ is estimable in the full model. Hence (5.30) is exactly the required condition on $[X_1', X_2']$, and is assumed in what follows.

An unbiased estimate of θ_1 in the full model can now be given as

$$\hat\theta_1=\tilde\theta_1-l_1'C_1X_1X_2'C_2X_2VY=l_1'\hat\beta_1.$$

Since θ and θ_1 are estimable in the full model, the same is true of

$$\theta_2=l_2'\beta_2=\theta-\theta_1,$$

so that

$$X_1d_2=0,\ X_2d_2=l_2$$

for some $n\times 1$ vector d_2. From this and (5.30) it can be verified that

$$\hat\theta_2=l_2'\hat\beta_2$$

is an estimate (therefore the best estimate) of θ_2 in the second-stage model, and also an unbiased estimate of θ_2 in the full model.

It has been shown that an unbiased estimate of the estimable function

$$\theta=l_1'\beta_1+l_2'\beta_2$$

is given by

$$\hat\theta=\hat\theta_1+\hat\theta_2=l_1'\hat\beta_1+l_2'\hat\beta_2,$$

where

$$\hat\beta_1=C_1[I+X_1X_2'C_2X_2X_1'C_1]X_1Y-C_1X_1X_2'C_2X_2Y,$$

$$\hat\beta_2=C_2X_2[I-X_1'C_1X_1]Y. \tag{5.31}$$

The solutions (5.31) can be shown by substitution to satisfy the normal equations

$$\begin{bmatrix}X_1X_1' & X_1X_2'\\ X_2X_1' & X_2X_2'\end{bmatrix}\begin{bmatrix}\hat\beta_1\\ \hat\beta_2\end{bmatrix}=\begin{bmatrix}X_1Y\\ X_2Y\end{bmatrix}$$

of the full model, and so $\hat\theta$ is the minimum variance linear unbiased estimate of θ.

For the same reason, $\hat\theta_i=l_i'\hat\beta_i$ is the best estimate of $\theta_i=l_i'\beta_i$ in the full model. In terms of this model alone, the following result has been proved: If the portions of every estimable function which respectively involve the β_1 and β_2 variables are separately estimable, then the best estimate of each such function is simply the sum of the best estimates of its portions. In this sense the condition (5.30) can be regarded as a generalization of orthogonality ($X_2X_1'=0$); in the orthogonal case the normal eqs (5.27) of the second-stage model are simply

$$(X_2X_2')\hat\beta_2=X_2Y$$

in direct analogy to those of the first-stage model. Note also that (5.30) automatically holds if $q=p$ (i.e., if A is nonsingular), since then every parametric function $l'\beta$, in particular $l_1'\beta_1$, is estimable.

5.6. Restraints Subject to Uncertainty

Occasionally situations arise in which the given restraints $K'\beta=m$ are themselves subject to variation. Such may be the case when the value of $K'\beta$ is not known but prior information is available which can be summarized as a value of a random vector $\hat m$ with $E(\hat m)=K'\beta$ and with precision described by var $(\hat m)=V_m\sigma^2$. A circumstance where this may occur is when data are available from another source which is believed to be without bias or systematic error.

Let $E(Y)=X'\beta$, var $Y=\sigma^2I$ and let the k "given" restraints consist of unbiased estimates $\hat m_i$ $(i=1,2)$ of $K_i'\beta$, where K_i is $p\times k_i$ of rank k_i, and $\hat m'=(\hat m_1', \hat m_2')$ obeys var $(\hat m)=V_m\sigma^2$. Further it is assumed that the restraints $K_1'\beta$ are nonpre-estimable functions and $K_2'\beta$ are pre-estimable functions with respect to the observational equations $E(Y)=X'\beta$. It is desired to perform estimation subject to the additional conditions $K_i'\hat\beta=\hat m_i$, i.e., to fit the new data so that the quantities $K'\beta$ are exactly equal to $\hat m$. We may assume without loss of generality that $K_2'K_2=I$ and that the restraints $K_1'\beta$ are irreducible.

It will be convenient to introduce the expression *undisturbed* to refer to those estimable functions $\theta=l'\beta$ whose best estimate $\hat\theta=l'\hat\beta$ is not altered by the requirement that $\hat\beta$ be chosen to satisfy $K'\hat\beta=\hat m$. Not all estimable functions are undisturbed in general; for example we have no freedom in choosing $\hat\theta$ when θ is a linear combination of the rows of $K_2'\beta$. The subclass of the estimable functions, consisting of those which are undisturbed, is a matter of *choice* and its selection would presumably depend on the problem at hand, but it should not contain any nonzero linear combinations of the rows of $K_2'\beta$. (If for example there is skepticism concerning the prior information, then this subclass would chosen to include, so far as possible, those functions for which a minimum variance estimate is of particular importance.) The class of undisturbed functions may be chosen, of the maximum possible dimension,

as the class of all linear combinations of the rows of $L'\beta$ where L is a $p\times(q-k_2)$ matrix of rank $q-k_2$ such that $H'L=0$ and $[K_2, L]$ has rank q. We may assume $L'L=I$ without loss of generality.

Because $H'[K_2, L]=0$, and $[K_2, L]$ has the same rank q as X, there exist a $k_2\times n$ matrix P_2 and a $(q-k_2)\times n$ matrix P such that

$$X=[K_2, L]\begin{bmatrix}P_2\\P\end{bmatrix}=K_2P_2+LP.$$

These matrices can be found explicitly, in terms of the inverse N^{-1} of the $q\times q$ nonsingular matrix

$$N=\begin{bmatrix}K_2'\\L'\end{bmatrix}[K_2, L]=\begin{bmatrix}I & K_2'L\\L'K_2 & I\end{bmatrix},$$

as

$$\begin{bmatrix}P_2\\P\end{bmatrix}=N^{-1}\begin{bmatrix}K_2'\\L'\end{bmatrix}X.$$

Since $E(\hat{m}_2)=K_2'\beta$, we find that $E(Y)=X'\beta$ is equivalent to

$$E(\overline{Y})=\overline{X}'\beta \tag{5.32}$$

where $\overline{Y}=Y-P_2'\hat{m}_2$ and $\overline{X}=LP=X-K_2P_2$. Similarly, under the assumption $\operatorname{cov}(Y, \hat{m}_2)=0$ which is implicit in our situation, it follows that $\operatorname{var}(Y)=\sigma^2I$ is equivalent to

$$\operatorname{var}(\overline{Y})=\overline{V}\sigma^2, \tag{5.33}$$

where $\overline{V}=I+P_2'V_2P_2$ and V_2 is defined by

$$\operatorname{var}(\hat{m}_2)=V_2\sigma^2.$$

Thus the original model $E(Y)=X'\beta$, $\operatorname{var} Y=\sigma^2I$, ignoring the restraint $K'\beta=\hat{m}$, is equivalent to the one given by (5.32) and (5.33).

From the fact that equality holds throughout the sequence

$$\begin{aligned}q=\operatorname{rank}(X)&=\operatorname{rank}(K_2P_2+LP)\\&\leqslant\operatorname{rank}(K_2P_2)+\operatorname{rank}(LP)\\&\leqslant\operatorname{rank}(K_2)+\operatorname{rank}(L)=k_2+(q-k_2)=q\end{aligned}$$

of inequalities, it follows in particular that $\overline{X}=LP$ has the same rank $q-k_2$ as L. Therefore the class of functions estimable with respect to (5.32) consists of all linear combinations of the rows of $L'\beta$.

We next prove that an analog of H for (5.32) is given by $\overline{H}=[H, (I-LL')K_2]$. Since $\overline{H}'\overline{X}=0$, it suffices to show that $\overline{H}$ has rank at least $p-(q-k_2)=r+k_2$; since

$$H'(I-LL')K_2=0$$

and H has rank r, it suffices to show that $(I-LL')K_2$ has at least rank k_2. This however follows from the consequence

$$\begin{bmatrix}I\\-L'K_2\end{bmatrix}=N^{-1}\begin{bmatrix}K_2'\\L'\end{bmatrix}(I-LL')K_2$$

of the identity

$$(I-LL')K_2=[K_2, L]\begin{bmatrix}I\\-L'K_2\end{bmatrix}.$$

From the irreducibility of the restraints $K_1'\beta$ in the original model, we can deduce that the restraints $K'\beta$, where $K=[K_1, K_2]$, are nonestimable and irreducible with respect to (5.32). Namely,

$$\overline{H}'K=\begin{bmatrix}H'K_1 & 0\\K_2'(I-LL')K_1 & K_2'(I-LL')K_2\end{bmatrix}$$

can be shown to have rank k_1+k_2. For this purpose, observe that $H'K_1$ has rank k_1 so that the same holds for the first block column in $\overline{H}'K$. Also, since $(I-LL')K_2$ has rank k_2, the same is true of

$$\{(I-LL')K_2\}'\{(I-LL')K_2\}=K_2'(I-LL')K_2$$

and thus of the second block column. The presence of the zero block then ensures the result.

Theorem 4 can be applied to the model consisting of (5.32) and (5.33), to obtain a new model analogous to (5.8), and the restraints $K'\beta$ will remain nonestimable in this new model. Thus the conditions $K'\hat{\beta}=\hat{m}$ can simply be adjoined to the normal equations of the new model without affecting the best estimates $\hat{\theta}$ of the functions estimable in this new model . . . i.e. the linear combinations of the rows of $L'\beta$. Thus, as desired, these linear forms have their best estimates "undisturbed" by requiring $K'\beta=\hat{m}$. (Here K plays the role of K_0 in Theorem 2.) If in particular $\overline{V}$ is nonsingular, then by Corollary 4.1 the normal equations become

$$(\overline{X}\overline{V}^{-1}\overline{X}')\hat{\beta}=\overline{X}\overline{V}^{-1}\overline{Y},$$

$$K'\hat{\beta}=\hat{m}.$$

It may also be appropriate to adjoin artificial nonpre-estimable restraints to secure a unique solution for β.

The previous material also permits us to arrive at unbiased estimates, consistent with $K'\hat{\beta}=\hat{m}$, of functions $\theta=l'\beta$ which are estimable in the original model but are *not* linear combinations of the rows of $L'\beta$. From

$$l=ACl=(K_2P_2+LP)X'Cl$$

it follows that

$$\theta=l'CXP_2'K_2'\beta+l'CXP'L'\beta,$$

so that an unbiased estimate is

$$\hat{\theta}=l'CXP_2'\hat{m}_2+l'CXP'L'\hat{\beta}=l'CX(P_2'K_2'+P'L')\hat{\beta}=l'\hat{\beta}$$

with $\hat{\beta}$ as in the last paragraph. Note that although the second summand $(l'CXP'L'\hat{\beta})$ in $\hat{\theta}$ is the best estimate of the second summand of θ, $\hat{\theta}$ as a whole does not coincide with the best estimate of θ in the original model since $\hat{\beta}$ comes from a set of normal

equations other than $A\hat{\beta} = XY$. Thus θ *has* been disturbed.

The previous material takes an especially simple form when $L'K_2 = 0$, i.e., when the estimable functions whose minimum-variance estimation is to be emphasized ($L'\beta$) are orthogonal to those whose estimates are prescribed ($K_2'\beta$). Here premultiplication of

$$X = K_2P_2 + LP$$

by K_2' and L', respectively, shows that $P_2 = K_2'X$ and $P = L'X$. Thus $\overline{H} = [H, K_2]$, and the model (5.32) and (5.33) becomes

$$E(\overline{Y}) = \overline{X}'\beta, \ \mathrm{var}(\overline{Y}) = \overline{V}\sigma^2$$

with

$$\overline{Y} = Y - X'K_2\hat{m}_2, \ \overline{X} = LL'X,$$

$$\overline{V} = I + X'K_2V_2K_2'X.$$

For a simple but artificial example, suppose

$$X = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \ K = K_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \ L = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

i.e., estimation of the second component β_2 of β is of principal importance. Suppose also that

$$\mathrm{var}(\hat{m}_2) = V_2\sigma^2 = \tau^2\sigma^2,$$

so that τ indicates the relative precision of the prior information relative to the new measurements under discussion. The previous paragraph applies, and we are led to the model

$$E(\overline{Y}) = \overline{X}'\beta, \ \mathrm{var}(\overline{Y}) = \overline{V}\sigma^2$$

with

$$\overline{Y} = \begin{bmatrix} y_1 - \hat{m}_2 \\ y_2 \end{bmatrix}, \ \overline{X} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix},$$

$$\overline{V} = \begin{bmatrix} 1+\tau^2 & 0 \\ 0 & 1 \end{bmatrix}.$$

This can be rewritten

$$E(\tilde{Y}) = \tilde{X}'\beta, \ \mathrm{var}(\tilde{Y}) = \sigma^2 I$$

with

$$\tilde{X} = \overline{X}, \ \tilde{Y}' = ((y_1 - \hat{m}_2)(1+\tau^2)^{-1/2}, y_2)'.$$

The normal equations of the new model are $(\tilde{X}\tilde{X}')\hat{\beta} = \tilde{X}\tilde{Y}$, i.e.,

$$0\hat{\beta}_1 + 0\hat{\beta}_2 = 0(y_1 - \hat{m}_2)(1+\tau^2)^{-1/2} + 0y_2,$$

$$0\hat{\beta}_1 + \hat{\beta}_2 = 0(y_1 - \hat{m}_2)(1+\tau^2)^{-1/2} + y_2,$$

to which we adjoin $K'\hat{\beta} = \hat{m}_2$, i.e., $\hat{\beta}_1 = \hat{m}_2$. Thus the result is

$$\hat{\beta}' = (\hat{m}_2, y_2)',$$

whereas without the requirement $K'\hat{\beta} = \hat{m}_2$ we would have

$$\hat{\beta}' = (y_1, y_2)'.$$

The estimate assigned to $\theta = \beta_1 + \beta_2$, which is not a linear combination of the rows of $L'\beta$, is

$$\theta = \hat{\beta}_1 + \hat{\beta}_2 = \hat{m}_2 + y_2$$

and has variance $\tau^2\sigma^2 + \sigma^2$, whereas the best estimate of θ in the original model is $y_1 + y_2$ with variance $2\sigma^2$. Thus the requirement $K'\hat{\beta} = \hat{m}_2$ decreases or increases the variance of the estimate of θ according as $\tau < 1$ or $\tau > 1$, i.e., according as the prior measurement of m_2 was more or less precise than the new measurement of y_1.

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(Paper 68B4–128)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 68B, No. 4, October–December 1964

Improvement of Bounds to Eigenvalues of Operators of the Form T^*T[1]

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(September 1, 1964)

The authors generalize a method of Lehmann and Maehly for upper and lower bounds to eigenvalues of self-adjoint operators in Hilbert space by using a device introduced by Kato. The resulting procedure can be used to improve bounds found by the Rayleigh-Ritz method and the comparison methods of Weinstein, Aronszajn, and the authors by means of calculations involving *easily found* vectors; and it is especially suitable for application to problems of vibration of continuous elastic systems. Further a theorem of Kato is interpreted and extended by the results obtained.

1. Introduction

For the eigenvalue problems that arise in the theory of vibration of continuous elastic systems it is useful to have auxiliary methods capable of improving the rigorous upper and lower bounds that can be found by the Rayleigh-Ritz and comparison operator procedures [1, 2, 3, 4][4]. We present here the theory of a method which should be quite useful in problems of this kind.

The procedure of Lehmann and Maehly [5, 6] is in principle applicable, since it depends on the use of an essentially arbitrary family of "trial vectors" and the knowledge of numbers that are known to separate adjacent eigenvalues. But while these numbers can be obtained by use of the upper and lower bound procedures already referred to, the trial vectors must satisfy all of the boundary conditions of the differential operators; and finding such vectors is far from an easy task. On the other hand Kato has developed [7] and applied [8] an extension of the Temple method [9] for operators of the form T^*T that uses the same numbers and avoids the difficulty of needing trial vectors that satisfy all of the boundary conditions. While the form T^*T is a common property of the operators that arise in elastic vibration theory, the procedure of Kato does not lend itself to optimization over a family of trial vectors. In the following lines we dicuss the use of a device introduced by Kato in the procedure of Lehmann and Maehly. The resulting procedure optimizes the estimate of Kato over a family of easily found trial vectors.

Section 2 sketches the needed properties of operators of the form T^*T and of the related operator H introduced by Kato. Section 3 then discusses the application of the procedure of Lehmann and Maehly to the operator H, and section 4 uses the results of section 3 to interpret and extend a theorem of Kato.

2. Operators of the Form T^*T and a Device of T. Kato

Here we are concerned with a positive self-adjoint operator A with domain $\mathfrak{D}_A$ in a Hilbert space $\mathfrak{H}^1$ for which the inner product is $(u, v)_1$. We will assume, for convenience, that the operator A has for its spectrum an infinite discrete set of eigenvalues, $0 \leq \lambda_1 \leq \lambda_2 \leq \ldots$, that diverge to infinity without finite limit points; i.e., that $(A+I)^{-1}$ is completely continuous. Further, we require A to have the form T^*T. The operator T is to be a closed operator defined on a dense domain $\mathfrak{D}_T$ in $\mathfrak{H}^1$ and having its range $\mathfrak{R}_T$ in a Hilbert space $\mathfrak{H}^2$ with inner product $(u, v)_2$; T^* is the operator adjoint to T. Thus, $\mathfrak{D}_{T^*}$ is in $\mathfrak{H}^2$, $\mathfrak{R}_{T^*}$ is in $\mathfrak{H}^1$, and together T and T^* satisfy $(Tu, v)_2 = (u, T^*v)_1$ for

[1] The research reported in this document has been sponsored in part by the Department of the Navy under Contract NOw-62-0604-c with the Bureau of Naval Weapons and in part by the Aeronautical Research Laboratories, OAR, through the European Office of Aerospace Research, United States Air Force.
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[4] Figures in brackets indicate the literature references at the end of this paper.

every u in $\mathfrak{D}_T$ and every v in $\mathfrak{D}_{T^*}$. The spaces $\mathfrak{H}^1$ and $\mathfrak{H}^2$ may possibly coincide. The properties of operators of the form T^*T have been widely studied by von Neumann [10], Murray [11], and others. Here we need draw on only a few of the properties of T, T^*, T^*T, and TT^*. We recall that the operators T^*T $(=A)$ and TT^* are positive self-adjoint operators which are isomorphic except for their null spaces $\mathfrak{N}_T$ and $\mathfrak{N}_{T^*}$ and that

$$\mathfrak{N}_T = \mathfrak{H}^1 \ominus \overline{\mathfrak{R}}_{T^*}, \qquad \mathfrak{N}_{T^*} = \mathfrak{H}^2 \ominus \overline{\mathfrak{R}}_T.$$

We define with Kato [7] the operator H in $\mathfrak{H}^1 \times \mathfrak{H}^2$ with inner product (u, v) given by $(u, v) = (u^1, v^1)_1 + (u^2, v^2)_2$ by

$$H[u^1, u^2] = [T^*u^2, Tu^1] \tag{1}$$

on all pairs $[u^1, u^2]$ in $\mathfrak{D}_T \times \mathfrak{D}_{T^*}$. H is a self-adjoint operator defined on $\mathfrak{D}_T \times \mathfrak{D}_{T^*}$ and has a real spectrum that is symmetric about zero. In fact, the unitary transformation U on $\mathfrak{H}^1 \times \mathfrak{H}^2$, defined by

$$U[u^1, u^2] = [u^1, -u^2], \tag{2}$$

transforms H into $-H$, that is,

$$-H = U^{-1}HU, \tag{3}$$

so that H and $-H$ are isomorphic. Further the operator H^2, which has the expression and domain given by

$$H^2[u^1, u^2] = [T^*Tu^1, TT^*u^2]$$

and

$$\mathfrak{D}_{H^2} = \mathfrak{D}_{T^*T} \times \mathfrak{D}_{TT^*},$$

respectively, is reduced by $\mathfrak{H}^1$ and $\mathfrak{H}^2$ regarded as subspaces of $\mathfrak{H}^1 \times \mathfrak{H}^2$. Evidently, $\mathfrak{N}_H = \mathfrak{N}_{H^2} = \mathfrak{N}_T \times \mathfrak{N}_{T^*}$. Excluding zero, H^2 has the same eigenvalues λ_ν as A but with the multiplicity doubled; since H is isomorphic with $-H$, it has just the nonzero numbers $+\lambda_\nu^{1/2}$ and $-\lambda_\nu^{1/2}$ as symmetrically arranged eigenvalues, each having the multiplicity of λ_ν in A. Thus the spectrum of H is completely described in terms of that of A with the possible addition of zero from $\mathfrak{N}_{T^*}$. On the other hand bounds for the eigenvalues of H can be converted into bounds for eigenvalues of A by squaring.

3. Application of the Lehmann-Maehly Procedure to the Operator H

In this section we apply the Lehmann-Maehly procedure to the operator H of section 2. We designate the *separation constant* by ρ or $-\rho$, where ρ is a non-negative real number. Our discussion considers first ρ in the resolvent set of H and then turns to ρ in the spectrum of H; finally, we consider what happens as ρ passes from the resolvent set to the spectrum.

The procedure of Lehmann and Maehly applied to a self-adjoint operator B makes use of a real constant τ that separates adjacent eigenvalues of B and amounts to the calculation of Rayleigh-Ritz bounds for the eigenvalues of the bounded operator $(B-\tau)^{-1}$ based on trial vectors φ of the form $\varphi = (B-\tau)v$, where the v's are linearly independent vectors from $\mathfrak{D}_B$. The resulting bounds are a consequence of the fact that for bounded operators the Rayleigh-Ritz method gives "inner bounds" for "outer eigenvalues".

3.1. ρ in the Resolvent Set of H

Let us suppose, at first, that ρ is a positive real number not in the spectrum of H. Then $-\rho$ is not in the spectrum of H, and $-\rho$ and ρ satisfy

$$-\lambda_{n+1}^{1/2} < -\rho < -\lambda_n^{1/2} \text{ and } \lambda_n^{1/2} < \rho < \lambda_{n+1}^{1/2},$$

respectively, for some [5] n. The operator $(H-\rho)^{-1}$ is bounded. The positive spectrum of $(H-\rho)^{-1}$

[5] We introduce the "conventional" eigenvalue λ_0 equal to zero whenever zero is not in the spectrum of A in order to unify the presentation.

consists of an infinite decreasing sequence of eigenvalues,

$$(\lambda_{n+1}^{1/2}-\rho)^{-1} \geq (\lambda_{n+2}^{1/2}-\rho)^{-1} \geq \ . \ . \ . \ > 0.$$

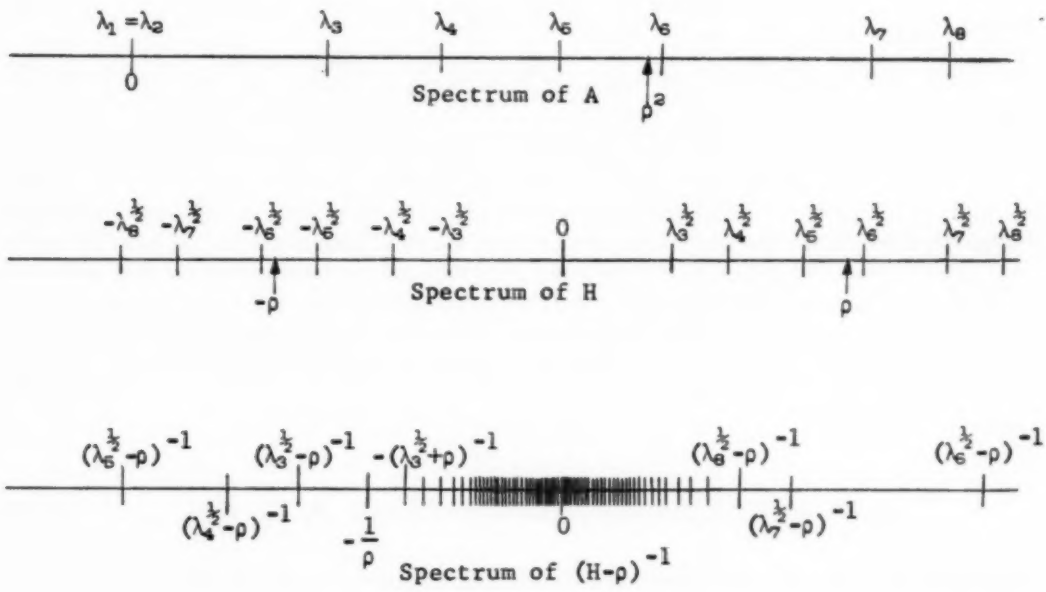
The negative spectrum begins with the increasing finite set (which is empty if $\lambda_n = \lambda_0 = 0$),

$$-(\rho-\lambda_n^{1/2})^{-1} \leq -(\rho-\lambda_{n-1}^{1/2})^{-1} \leq \ . \ . \ . \ \leq -(\rho-\lambda_p^{1/2})^{-1},$$

where λ_p designates the first nonzero eigenvalue of A; the point $-1/\rho$ has an associated characteristic subspace equal to $\mathfrak{N}_H$; and the interval $(-1/\rho, 0)$ contains the infinite set of negative eigenvalues,

$$-(\rho+\lambda_p^{1/2})^{-1} \leq -(\rho+\lambda_{p+1}^{1/2})^{-1} \leq \ . \ . \ . \ < 0.$$

The following spectral diagrams may be helpful. For the sake of illustration we have assumed $\rho = 3$ so that $\lambda_1 = \lambda_2 = 0$, $\lambda_3 > 0$ and $\lambda_3 < \rho^2 < \lambda_6$.



The operator $(H+\rho)^{-1}$ is also bounded and has the same norm as $(H-\rho)^{-1}$. In fact, since H and $-H$ are isomorphic, it follows that $(H+\rho)^{-1}$ is isomorphic with $-(H-\rho)^{-1}$, so that the spectrum of $(H+\rho)^{-1}$ is the same as that of $(H-\rho)^{-1}$ after a reflection about the origin.

The Lehmann-Maehly procedure can be applied to H using ρ or $-\rho$ as the separating constant. If we use ρ and base the procedure on an m^+-dimensional manifold $\mathfrak{M}^+$ of $\mathfrak{D}_H$, then the resulting eigenvalues, designated by μ^+, are the stationary values over vectors v in $\mathfrak{M}^+$ of the ratio

$$\frac{((H-\rho)v,\ v)}{((H-\rho)v,\ (H-\rho)v)},$$

and may be determined from a matrix eigenvalue equation of the form

$$(A-\mu^+ B)\alpha = 0.$$

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The matrices A and B are given in terms of a linearly independent basis $\{v_i\}$ for $\mathfrak{M}^+$ by

$$A=\{((H-\rho)v_i, v_j)\} \text{ and } B=\{((H-\rho)v_i, (H-\rho)v_j)\}.$$

Let us agree to enumerate the nonzero eigenvalues by the useful but unconventional scheme,

$$\mu_n^+ \leqslant \mu_{n-1}^+ \leqslant \ldots \leqslant \mu_{n+1-j^+}^+ < -\frac{1}{\rho} \leqslant \mu_{p-s}^+ \leqslant \mu_{p-s+1}^+ \leqslant \ldots \leqslant \mu_{p+k^+-s-1}^+ < 0,$$

and

$$0<\mu_{n+l^+}^+ \leqslant \ldots \leqslant \mu_{n+2}^+ \leqslant \mu_{n+1}^+,$$

where s is the dimension (possibly infinite) of $\mathfrak{N}_H$, and the quantities j^+, k^+, and l^+ are nonnegative integers that satisfy $j^+ \leqslant n-p+1$ and $j^+ + k^+ + l^+ \leqslant m^+$. Since the negative eigenvalues give upper bounds to the negative eigenvalues of $(H-\rho)^{-1}$ and the positive give lower bounds to the positive, we have [6]

$$\mu_r^+ \geqslant (\lambda_r^{1/2}-\rho)^{-1}, \qquad r=n, n-1, \ldots, n+1-j^+, \tag{4}$$

$$\mu_r^+ \geqslant -(\lambda_r^{1/2}+\rho)^{-1}, \qquad r=p, p+1, \ldots, p+k^+-s-1, \tag{5}$$

and

$$\mu_r^+ \leqslant (\lambda_r^{1/2}-\rho)^{-1}, \qquad r=n+1, n+2, \ldots, n+l^+, \tag{6}$$

or equivalently,

$$\lambda_r^{1/2} \geqslant \rho+\frac{1}{\mu_r^+}, \qquad r=n, n-1, \ldots, n+1-j^+, \tag{7}$$

$$-\lambda_r^{1/2} \geqslant \rho+\frac{1}{\mu_r^+}, \qquad r=p, p+1, \ldots, p+k^+-s-1, \tag{8}$$

and

$$\lambda_r^{1/2} \leqslant \rho+\frac{1}{\mu_r^+}, \qquad r=n+1, n+2, \ldots, n+l^+. \tag{9}$$

When they are squared, the inequalities (7), (8), and (9) give lower bounds for λ_n, λ_{n-1}, . . ., λ_{n+1-j^+} and upper bounds for λ_p, λ_{p+1}, . . ., λ_{p+k^+-s-1}, and for λ_{n+1}, λ_{n+2}, . . ., λ_{n+l^+}.

If $-\rho$ is used in place of ρ in the Lehmann-Maehly procedure on H, we designate the eigenvalues based on an m^--dimensional subspace $\mathfrak{M}^-$ in $\mathfrak{D}_H$ by μ^- and enumerate those that are nonzero according to

$$\mu_{n+1}^- \leqslant \mu_{n+2}^- \leqslant \ldots \leqslant \mu_{n+l^-}^- < 0,$$

and

$$0<\mu_{p+k^--s-1}^- \leqslant \ldots \leqslant \mu_{p-s+1}^- \leqslant \mu_{p-s}^- \leqslant \frac{1}{\rho} < \mu_{n+1-j^-}^- \leqslant \ldots \leqslant \mu_{n-1}^- \leqslant \mu_n^-,$$

---

[6] We omit the valid but useless bounds $\mu_n^+ \geqslant -\frac{1}{\rho}$, $n=p-s, p-s+1, \ldots, p-1$ and note that (5) gives useful information only when s is finite and $k^+ > s$.

where j^-, k^-, and l^- are nonnegative integers that satisfy $j^- \leq n-p+1$ and $j^-+k^-+l^- \leq m^-$. By arguments parallel with those for ρ we find the bounds

$$\lambda_r^{1/2} \geq \rho - \frac{1}{\mu_r^-}, \qquad r=n, n-1, \ldots, n+1-j^-, \tag{10}$$

$$-\lambda_r^{1/2} \geq \rho - \frac{1}{\mu_r^-}, \qquad r=p, p+1, \ldots, p+k^--s-1, \tag{11}$$

and

$$\lambda_r^{1/2} \leq \rho - \frac{1}{\mu_r^-}, \qquad r=n+1, n+2, \ldots, n+l^-. \tag{12}$$

When squared, these inequalities give lower bounds for $\lambda_n, \lambda_{n-1}, \ldots, \lambda_{n+1-j^-}$, and upper bounds for $\lambda_p, \lambda_{p+1}, \ldots, \lambda_{p+k^--s-1}$ and for $\lambda_{n+1}, \lambda_{n+2}, \ldots, \lambda_{n+l^-}$.

Although, in general, the bounds given by the procedure using ρ will differ from those obtained using $-\rho$, even when the manifolds $\mathfrak{M}^+$ and $\mathfrak{M}^-$ are the same, there is an important case in which they will be identical. This happens when

$$U\mathfrak{M}^+ = \mathfrak{M}^-, \tag{13}$$

where U is the unitary transformation given by (2), as is clear from the equality,

$$\frac{((H-\rho)v, v)}{((H-\rho)v, (H-\rho)v)} = -\frac{((H+\rho)Uv, Uv)}{((H+\rho)Uv, (H+\rho)Uv)},$$

that follows from (3). In fact, when (13) holds we have $\mu_r^+ = -\mu_r^-$, and $j^+ = j^-$, $k^+ = k^-$, and $l^+ = l^-$. When $\mathfrak{M}^+$ and $\mathfrak{M}^-$ are equal and (13) is satisfied, then it is always possible to choose a basis $\{v_i\}$ such that each vector has the form $[v^1, 0]$ or $[0, v^2]$, as is evident from the definition (2) of U.

No matter whether ρ or $-\rho$ is used, the bounds given on the right hand sides of (7), (8), (9), (10), (11), and (12) are increasing with ρ. In fact, if we designate a right hand side of an inequality (7), (8) or (9) by ω^+, then it follows from the stationary property of μ^+ that ω^+ is a stationary value of the quotient

$$\frac{((H-\rho)v, Hv)}{((H-\rho)v, v)} \tag{14}$$

over the vectors of $\mathfrak{M}^+$, and that a vector v^+ that makes the quotient stationary gives

$$\omega^+ = \frac{((H-\rho)v^+, Hv^+)}{((H-\rho)v^+, v^+)}.$$

When the eigenvalues ω^+ and corresponding eigenvectors v^+ are considered as functions of ρ they are analytic.[7] Considering the variation of a ω^+ with respect to ρ we find that

$$\frac{d\omega^+}{d\rho} = \frac{(Hv^+, Hv^+)(v^+, v^+) - (Hv^+, v^+)^2}{((H-\rho)v^+, v^+)^2} \geq 0.$$

In computing this derivative the contribution from the variation of v^+ with ρ is zero since the ratio (14) is stationary at v^+. Similarly, for ω^-, a right hand side in (10), (11), or (12), we find

$$\dot{\omega}^- = -\frac{((H+\rho)v^-, Hv^-)}{((H+\rho)v^-, v^-)},$$

[7] Strictly speaking, it may be necessary in order to preserve their analyticity in ρ to rename the eigenvalues and eigenvectors in neighborhoods of ρ where they are multiple. This in no way affects the validity of the argument since all the ω^+'s are nondecreasing in ρ.

and

$$\frac{d\omega^-}{d\rho} = \frac{(Hv^-, Hv^-)(v^-, v^-) - (Hv^-, v^-)^2}{((H+\rho)v^-, v^-)^2} \geq 0.$$

Since all of the bounds are increasing with ρ, the best lower bounds will be obtained when ρ^2 is the largest known lower bound to λ_{n+1}; and, conversely, the best upper bounds will be taken when ρ^2 is the smallest known upper bound to λ_n.

3.2. ρ in the Spectrum of H

Let us now suppose that ρ coincides with an eigenvalue of H. Our considerations can be conveniently divided into the two cases: $\rho = 0$ and $\rho > 0$. (The results for $-\rho$ follow analogously to those for ρ.)

If ρ is zero then the Lehmann-Maehly procedure can be applied to the restriction of H to the orthogonal complement of the null space $\mathfrak{N}_H$. As we shall see, this produces upper bounds for the *strictly positive* eigenvalues of A, but these upper bounds may not be as good as those obtained from the usual Rayleigh-Ritz procedure based on essentially the same family of trial vectors. Let us designate the restriction of H to the orthogonal complement of $\mathfrak{N}_H$ by H^0 and the orthogonal projection on this complement by P^0. We apply the procedure using an m^0-dimensional manifold $\mathfrak{M}^0$ of $\mathfrak{D}_{H^0}$. Let us designate the resulting nonzero eigenvalues according to

$$\mu_p^0 \leq \mu_{p+1}^0 \leq \ldots \leq \mu_{p+t_1-1}^0 < 0 < \tilde{\mu}_{p+t_2-1}^0 \leq \ldots \leq \tilde{\mu}_{p+1}^0 \leq \tilde{\mu}_p^0,$$

where t_1 and t_2 are nonnegative integers that satisfy $t_1 + t_2 \leq m^0$. Since the negative eigenvalues are upper bounds to the negative eigenvalues of $(H^0)^{-1}$ and the positive to the positive, we have

$$\lambda_r^{1/2} \leq -\frac{1}{\mu_r^0}, \qquad r = p, p+1, \ldots, p+t_1-1, \tag{15}$$

and

$$\lambda_r^{1/2} \leq \frac{1}{\tilde{\mu}_r^0}, \qquad r = p, p+1, \ldots, p+t_2-1. \tag{16}$$

Further, if $U\mathfrak{M}^0 = \mathfrak{M}^0$ we have $t_1 = t_2$ and $\tilde{\mu}_r^0 = -\mu_r^0$, as follows from (3).

It is important to note that to apply the Lehmann-Maehly procedure with ρ equal to zero, it is no way necessary to know explicitly the operators H^0 or P^0 or to find vectors orthogonal to $\mathfrak{N}_H$. In fact, if $\tilde{\mathfrak{M}}^0$ is any m^0-dimensional manifold in $\mathfrak{D}_H$ for which rank $\{(Hv_i, Hv_j)\} = m^0$, where $\{v_i\}$ is a basis for $\tilde{\mathfrak{M}}^0$, then the manifold $\mathfrak{M}^0$ given by $P^0\tilde{\mathfrak{M}}^0$ is of dimension m^0 as well and lies in the orthogonal complement of $\mathfrak{N}_H$. Further, the inner products used in the procedure are just (Hv_i, v_j) and (Hv_i, Hv_j), as follows from the relation $P^0H^0P^0 = H^0 = H$ on $\mathfrak{D}_H$.

If A has no zero eigenvalues, then the upper bounds given by (15) and (16) are always weaker than those given by the usual Rayleigh-Ritz procedure for A based on the projection of $\tilde{\mathfrak{M}}^0$ on $\mathfrak{H}^1$. In fact, we may assume that $\tilde{\mathfrak{M}}^0$ satisfies $U\tilde{\mathfrak{M}}^0 = \tilde{\mathfrak{M}}^0$, for if it does not, we can replace it by the even larger space obtained by forming $\tilde{\mathfrak{M}}^0 + U\tilde{\mathfrak{M}}^0$ and then removing the submanifold that lies in $\mathfrak{N}_H$. The bounds obtained from the enlarged space will be better than those given by (10) and (11), and they will be symmetrically arranged about the origin. As we shall see, the Rayleigh-Ritz bounds will be even better. Let us suppose, then, that $\tilde{\mathfrak{M}}^0$ satisfies $U\tilde{\mathfrak{M}}^0 = \tilde{\mathfrak{M}}^0$ and that a basis is taken using vectors of the form $[v^1, 0]$ and $[0, v^2]$. Those of the first set form a basis for the projection of $\tilde{\mathfrak{M}}^0$ on $\mathfrak{H}^1$, and those of the second for the projection of $\tilde{\mathfrak{M}}^0$ on $\mathfrak{H}^2$ after removal of the part in $\mathfrak{N}_H$. The matrix eigenvalue problem takes the form

$$\left\{ \left(\begin{array}{c|c} 0 & C \\ \hline C^* & 0 \end{array} \right) - \mu \left(\begin{array}{c|c} B_1 & 0 \\ \hline 0 & B_2 \end{array} \right) \right\} \left(\begin{array}{c} \alpha^1 \\ \hline \alpha^2 \end{array} \right) = 0, \tag{17}$$

where B_1 and B_2 are the positive definite matrices given by

$$B_1 = \{(Tv_i^1, Tv_j^1)_2\}, \qquad \text{and } B_2 = \{(T^*v_i^2, T^*v_j^2)_1\},$$

and C and C^* are the matrices given by

$$C = \{(Tv_i^1, v_j^2)_2\}, \qquad \text{and } C^* = \{(T^*v_i^2, v_j^1)_1\}.$$

But the matrix equation (17) has just the same nonzero eigenvalues as the equation

$$(CB_2^{-1}C^* - \mu^2 B_1)\alpha^1 = 0. \tag{18}$$

However, since the matrix $CB_2^{-1}C^*$ is the Gram matrix of the orthogonal projection in $\mathfrak{H}^1$ of the vectors $\{v_i^1\}$ on the subspace spanned by the vectors $\{T^*v_i^2\}$, we have the matrix inequality,

$$CB_2^{-1}C^* \leqslant \Gamma,$$

in which Γ is the Gram matrix of the vectors $\{v_i^1\}$. Thus, according to the minimum-maximum principle, the eigenvalues, $\hat{\mu}_1^2 \geqslant \hat{\mu}_2^2 \geqslant \ldots$, of the matrix equation

$$(\Gamma - \hat{\mu}^2 B_1)\alpha^1 = 0 \tag{19}$$

are larger than those of (18). That is,

$$(\mu_i^0)^2 \leqslant \hat{\mu}_i^2, \qquad i = 1, 2, \ldots, t,$$

and hence,

$$\lambda_i \leqslant \frac{1}{\hat{\mu}_i^2} \leqslant \frac{1}{(\mu_i^0)^2}, \qquad i = 1, 2, \ldots, t.$$

But the matrix equation (19) is just that which arises from the Rayleigh-Ritz procedure for A using the projection of $\tilde{\mathfrak{M}}^0$ on $\mathfrak{H}^1$.

If, however, A has zero in its spectrum, our conclusion is no longer valid, for the Rayleigh-Ritz procedure gives upper bounds starting with the lowest, which is zero, while the Lehmann-Maehly procedure starts with the first *strictly positive* eigenvalue.

When ρ is equal to a nonzero eigenvalue of H, that is, $0 < \rho = \lambda_\nu^{1/2}$, we proceed in much the same way as for ρ equal to zero. Suppose λ_ν is an eigenvalue of A of multiplicity t, i.e.,

$$\lambda_{\nu-1} < \lambda_\nu = \lambda_{\nu+1} = \ldots = \lambda_{\nu+t-1} < \lambda_{\nu+t}, \tag{20}$$

and that $\mathfrak{N}_\nu^+$ is the characteristic subspace associated with $\lambda_\nu^{1/2}$ as an eigenvalue of H. We designate by H_ν^+ the restriction of H to the orthogonal complement of $\mathfrak{N}_\nu^+$ and apply to it the procedure using ρ and an m_ν^+-dimensional manifold $\mathfrak{M}_\nu^+$ of vectors in $\mathfrak{D}_{H_\nu^+}$. The negative eigenvalues less than $-1/\rho$ of the procedure give rise to lower bounds for eigenvalues of H_ν^+ below ρ. Since the spectrum of H_ν^+ coincides with that of H after the omission of $\lambda_\nu^{1/2}$, we find bounds to eigenvalues of A. Designating the nonzero eigenvalues according to

$$\mu_{\nu-1}^{+\nu} \leqslant \mu_{\nu-2}^{+\nu} \leqslant \ldots \leqslant \mu_{\nu-j_\nu^+}^{+\nu} < -\frac{1}{\rho} \leqslant \mu_{p-s}^{+\nu} \leqslant \mu_{p-s+1}^{+\nu} \leqslant \ldots \leqslant \mu_{p+k_\nu^+-s-1}^{+\nu} < 0$$

and

$$0 < \mu_{\nu+t+l_\nu^+-1}^{+\nu} \leqslant \ldots \leqslant \mu_{\nu+t+1}^{+\nu} \leqslant \mu_{\nu+t}^{+\nu},$$

where j_ν^+, k_ν^+, and l_ν^+ are nonnegative integers that satisfy $j_\nu^+ \leq \nu - p$, $j_\nu^+ + k_\nu^+ + l_\nu^+ \leq m_\nu^+$, we obtain the bounds

$$\lambda_r^{\nu} \geq \rho + \frac{1}{\mu_r^{+\nu}}, \qquad r = \nu - 1, \nu - 2, \ldots, \nu - j_\nu^+, \tag{21}$$

$$-\lambda_r^{\nu} \geq \rho + \frac{1}{\mu_r^{+\nu}}, \qquad r = p, p+1, \ldots, p + k_\nu^+ + s - 1, \tag{22}$$

and

$$\lambda_r^{\nu} \geq \rho + \frac{1}{\mu_r^{+\nu}}, \qquad r = \nu + t, \nu + t + 1, \ldots, \nu + t + l_\nu^+ - 1. \tag{23}$$

Parallelly, using $-\rho$ we find bounds in terms of the eigenvalues,

$$\mu_{\nu+t}^{-\nu} \leq \mu_{\nu+t+1}^{-\nu} \leq \ldots \leq \mu_{\nu+t+l_\nu^- - 1}^{-\nu} < 0,$$

and

$$0 < \mu_{p+k_\nu^- - s - 1}^{-\nu} \leq \ldots \leq \mu_{p-s+1}^{-\nu} \leq \mu_{p-s}^{-\nu} \leq \frac{1}{\rho} < \mu_{\nu - j_\nu^-}^{-\nu} \leq \ldots \leq \mu_{\nu-2}^{-\nu} \leq \mu_{\nu-1}^{-\nu},$$

according to

$$\lambda_r^{\nu} \geq \rho - \frac{1}{\mu_r^{-\nu}}, \qquad r = \nu - 1, \nu - 2, \ldots, \nu - j_\nu^-, \tag{24}$$

$$-\lambda_r^{\nu} \geq \rho - \frac{1}{\mu_r^{-\nu}}, \qquad r = p, p+1, \ldots, p + k_\nu^- - s - 1, \tag{25}$$

and

$$\lambda_r^{\nu} \leq \rho - \frac{1}{\mu_r^{-\nu}}, \qquad r = \nu + t, \nu + t + 1, \ldots, \nu + t + l_\nu^- - 1. \tag{26}$$

As in the previous cases, we find that $\mu_r^{+\nu} = \mu_r^{-\nu}$ provided that $U\mathfrak{M}_\nu^+ = \mathfrak{M}_\nu^-$. The characteristic subspace $\mathfrak{N}_\nu^+$ does not need to be known, nor do vectors orthogonal to it have to be found explicitly. In fact, if $\tilde{\mathfrak{M}}_\nu^+$ is an m_ν^+-dimensional manifold in $\mathfrak{D}_H$ that satisfies rank $\{((H-\rho)v_i, (H-\rho)v_j)\} = m_\nu^+$ for a basis $\{v_i\}$ for $\tilde{\mathfrak{M}}_\nu^+$, then $\tilde{\mathfrak{M}}_\nu^+$ can be used in place of $\mathfrak{M}_\nu^+$, and the inner products needed are just $((H-\rho)v_i, (H-\rho)v_j)$ and $((H-\rho)v_i, v_j)$.

The manifolds $\mathfrak{M}$ that we have introduced when ρ is in the spectrum of H have the advantage that in each case the eigenvalue problem has the matrix form, $(A - \mu B)\alpha = 0$, in which B is positive definite. This restriction is not really necessary. The eigenvalues may be defined to be stationary values of the quotient.

$$\frac{((H-\rho)v, v)}{((H-\rho)v, (H-\rho)v)}$$

over vectors v in an arbitrary m-dimensional manifold $\mathfrak{M}$ of $\mathfrak{D}_H$ under the subsidiary condition that $((H-\rho)v, (H-\rho)v) > 0$. In fact, the eigenvalues may be defined[8] as recursive maxima or minima or by minimum-maxima or maximum-minima of $((H-\rho)v, v)$ under the condition $((H-\rho)v, (H-\rho)v) = 1$. Evidently the eigenvalues μ are uniquely defined and are equivalent to those found using only that part of $\mathfrak{M}$ in the orthogonal complement of $\mathfrak{N}$, while the eigenvectors in $\mathfrak{M}$ are undetermined to the extent of an arbitrary vector v in $\mathfrak{M} \cap \mathfrak{N}$.

[8] The orthogonality statements in the variational principles are to be understood in terms of the form $((H-\rho)v, (H-\rho)v)$.

3.3. ρ Passes From the Resolvent Set to the Spectrum

We now examine what happens when ρ passes from the resolvent set of H to a point σ of the spectrum. We shall see that the bounds pass smoothly, indeed analytically, into those given at the spectral point. In order to preserve the proper enumeration, and thus obtain the strongest bounds, it is necessary to consider the limits from both sides of the spectral point.

Let σ be a nonnegative point of the spectrum of H and let $\mathfrak{N}^\sigma$ be the associated characteristic subspace. We take $\mathfrak{M}$ to be an m-dimensional subspace of $\mathfrak{D}_H$ and suppose that $\{v_i\}$ is an orthonormal basis for $\mathfrak{M}$ such that $v_i \epsilon \mathfrak{N}^\sigma$, $i = m'+1, m'+2, \ldots, m$, and that the other vectors in the basis have no nontrivial linear combinations in $\mathfrak{N}^\sigma$. The manifold spanned by the first m' of the v's will be denoted by $\tilde{\mathfrak{M}}_\sigma$. We restrict our attention to ρ's that are distinct from σ and lie in an interval about σ that contains no other spectral points of H. The Lehmann-Maehly eigenvalue equation for H based on ρ and $\mathfrak{M}$ takes the form,

$$\left\{\begin{pmatrix} A_1(\rho) & 0 \\ 0 & (\sigma-\rho)I \end{pmatrix} - \mu \begin{pmatrix} B_1(\rho) & 0 \\ 0 & (\sigma-\rho)^2 I \end{pmatrix}\right\}\begin{pmatrix} \alpha^1 \\ \alpha^2 \end{pmatrix} = 0,$$

in which A_1 and B_1 are given by $((H-\rho)v_i, v_j)$ and $((H-\rho)v_i, (H-\rho)v_j)$, respectively, $i, j = 1, 2, \ldots, m'$. Equivalently, we have

$$(A_1 - \mu B_1)\alpha^1 = 0, \tag{27}$$

and

$$\{I - \mu(\sigma-\rho)\}\alpha^2 = 0. \tag{28}$$

As ρ approaches σ the values μ determined by (28) become infinite while the numbers $\rho + 1/\mu$ have the constant value σ. The μ's determined by (27) depend analytically on ρ and pass to the values found with ρ equal to σ.

Let us assume that σ is $\lambda_\nu^{1/2}$, where λ_ν is the same as in (20). We identify $\mathfrak{M}$ with $\mathfrak{M}^+$, $\tilde{\mathfrak{M}}_\sigma$ with $\tilde{\mathfrak{M}}_\nu^+$, m with m^+ and m' with m_ν^+. As ρ approaches $\lambda_\nu^{1/2}$ from above the bounds given by (8) decrease to those of (22) and the bounds given by (9) with n equal to $\nu + t - 1$ decrease to those of (23).[9] The numbers obtained as the limiting values of the right side of (7) contain $\lambda_\nu^{1/2}$ repeated $m - m'$ times and the others are the bounds found on the right hand side of (21), but the enumeration obtained by the limiting process will not be as strong as that in (21) unless $m - m'$ equals t. On the other hand as ρ increases to $\lambda_\nu^{1/2}$ the bounds given by (7) with n equal to $\nu - 1$ and by (8) increase with ρ to those given by (21) and (22) respectively. The numbers obtained as the limits of the right hand side of (9) will contain $\lambda_\nu^{1/2}$ repeated $m - m'$ times and the others are the bounds found on the right hand side of (23). Again, if $m - m'$ is less than t, the enumeration of the bounds found from (9) by the limiting process will not be as strong as that of (23). Evidently, a parallel discussion can be made for the bounds found with $-\rho$ to relate the limiting values of the bounds of (10), (11), and (12) to those of (24), (25), and (26).

If we assume that σ is zero, we identify $\mathfrak{M}$ with $\mathfrak{M}^+$, $\tilde{\mathfrak{M}}_\sigma$ with $\tilde{\mathfrak{M}}^0$, m with m^+ and m' with m^0. As ρ approaches zero from above the bounds given by (9) with n equal to $p - 1$ decrease to those of (16). The set of bounds given by (7) is empty, and the limiting values of the right-hand side of (8) contain zero repeated $m - m'$ times and the others are the numbers that appear on the right in (15), but the enumeration obtained in the limit will not be as strong as that of (15) unless $m - m'$ equals s. To obtain the bounds (15) directly as limits we use $-\rho$. For this we identify $\mathfrak{M}$ with $\mathfrak{M}^-$ and m with m^-. As ρ approaches zero from above, the bounds of (12) with n equal to $p - 1$ decrease to those of (15). The set of bounds given by (11) is empty, and the limiting values of the right hand side of (10) contain zero $m - m'$ times and those of the right hand side of (16). Again precise enumeration is lost unless $m - m'$ equals s.

[9] The numbers j^+, k^+, and l^+ change with ρ as values of μ pass through zero or $-1/\rho$.

4. An Interpretation of a Theorem of T. Kato

T. Kato [7], has proved the following theorem:

Let H *be the operator described in sec. 2, and suppose that the interval* (α,β), $0 \leq \alpha < \beta$, *contains at most a nondegenerate eigenvalue of* H. *If* v, *a nonzero vector in* $\mathfrak{D}_H$, *satisfies*

$$\epsilon^2 < (\eta-\alpha)(\beta-\eta), \tag{29}$$

where

$$\eta = \frac{(\mathrm{Hv}, \mathrm{v})}{(\mathrm{v},\mathrm{v})} \text{ and } \epsilon^2 = \frac{(\mathrm{Hv}, \mathrm{Hv})}{(\mathrm{v},\mathrm{v})} - \eta^2,$$

then there is an eigenvalue $\lambda^{1/2}$ *of* H *in* (α,β) *and the following bounds hold:*

$$\alpha < \eta - \frac{\epsilon^2}{\beta-\eta} \leq \lambda^{1/2} \leq \eta + \frac{\epsilon^2}{\eta-\alpha} < \beta. \tag{30}$$

We first note that the inequality (29) is equivalent to each of the inequalities

$$\frac{((H-\beta)v,\, v)}{((H-\beta)v,\, (H-\beta)v)} < \frac{-1}{\beta-\alpha}, \tag{31}$$

and

$$\frac{((H-\alpha)v,\, v)}{((H-\alpha)v,\, (H-\alpha)v)} < \frac{1}{\beta-\alpha}, \tag{32}$$

and that the bounds (30) can be written

$$\alpha < \beta + \frac{((H-\beta)v,\, (H-\beta)v)}{((H-\beta)v,\, v)} \leq \lambda^{1/2} \leq \alpha + \frac{((H-\alpha)v,\, (H-\alpha)v)}{((H-\alpha)v,\, v)} < \beta. \tag{33}$$

From the form of the bounds in (33) it is clear that the theorem of Kato can be interpreted as the application of the Lehmann-Maehly procedure based on the one-dimensional manifold spanned by v and using in turn α and β as ρ. The inequality (29) suffices to insure that the bounds give improvements over α and β. Further, the procedure applied to H using a fixed finite-dimensional manifold $\mathfrak{M}$ and the constants α and β gives the best possible bounds [10] of the Kato type (33) that can be obtained using v's from $\mathfrak{M}$. In fact, the smallest eigenvalue $\mu(\beta)$ of the procedure based on $\mathfrak{M}$ and β is the minimum of the quotient $\dfrac{((H-\beta)v,\, v)}{((H-\beta)v,\, (H-\beta)v)}$ over $\mathfrak{M}$, and if there is any v in $\mathfrak{M}$ that satisfies (29) then it satisfies (31), which guarantees that

$$\mu(\beta) < \frac{-1}{\beta-\alpha}.$$

In addition, we have by the minimum property of $\mu(\beta)$ that

$$\mu(\beta) \leq \frac{((H-\beta)v,\, v)}{((H-\beta)v,\, (H-\beta)v)}$$

for any v in $\mathfrak{M}$ for which $(H-\beta)v \neq 0$. Consequently, any lower bound of the form $\beta + \dfrac{((H-\beta)v,\, (H-\beta)v)}{((H-\beta)v,\, v)}$ can be no better than that given by $\beta + \dfrac{1}{\mu(\beta)}$, which shows that the Lehmann-Maehly procedure is optimum for the lower bound. Similarly, the largest eigenvalue $\mu(\alpha)$ of the procedure based on α and $\mathfrak{M}$ is the maximum value of the quotient $\dfrac{((H-\alpha)v,\, v)}{((H-\alpha)v,\, (H-\alpha)v)}$, and by (32) it satisfies

$$\mu(\alpha) > \frac{1}{\beta-\alpha}.$$

[10] Kato suggested [7] and used [8] a process that tends to minimize ϵ^2 instead.

The maximum characterization yields

$$\mu(\alpha) \geq \frac{((H-\alpha)v,\, v)}{((H-\alpha)v,\, (H-\alpha)v)}$$

for any v in $\mathfrak{M}$ for which $(H-\alpha)v \neq 0$, and thus the procedure yields the best upper bound of the form $\alpha + \dfrac{((H-\alpha)v,\, (H-\alpha)v)}{((H-\alpha)v,\, v)}$. According to the equivalence of the inequalities (31) and (32), a vector v_β that yields $\mu(\beta)$ less than $-(\beta-\alpha)^{-1}$ satisfies (31) and hence (32), and conversely a vector v_α that yields $\mu(\alpha)$ greater than $(\beta-\alpha)^{-1}$ satisfies (32) and thus (31). Nevertheless, the vectors v_α and v_β will be different in general, even when neither α nor β is in the spectrum of H; that is to say that the upper and lower bounds are optimized separately by the procedure of Lehmann and Maehly.

Let us note that it is not necessary to assume that the interval (α, β) contains at most one eigenvalue of H. In fact, if the procedure based on $\mathfrak{M}$ and β yields j^+ eigenvalues $\mu_r(\beta)$ that are less than $-(\beta-\alpha)^{-1}$ then from these μ's there result j^+ positive lower bounds of the form $\beta + \dfrac{1}{\mu_r(\beta)}$ for the eigenvalues of H that lie just below β, and these bounds satisfy

$$\alpha < \beta + \frac{1}{\mu_r(\beta)} < \beta.$$

Consequently, there are at least j^+ eigenvalues of H in the interval $[\beta + (\min \mu_r(\beta))^{-1}, \beta)$. However, since the inequality (31) is equivalent to (32), the procedure for H based on $\mathfrak{M}$ and α has also exactly j^+ eigenvalues $\mu_r(\alpha)$ greater than $(\beta-\alpha)^{-1}$. These give j^+ upper bounds of the form $\alpha + \dfrac{1}{\mu_r(\alpha)}$ for the eigenvalues of H that lie just above α, and they satisfy

$$\alpha < \alpha + \frac{1}{\mu_r(\alpha)} < \beta.$$

Hence there are also at least j^+ eigenvalues of H in the interval $(\alpha, \alpha + (\max \mu_r(\alpha))^{-1}]$. If it is known that there are at most j^+ eigenvalues of H in (α, β), then the results from the use of α and β combine to assert that there are exactly j^+ eigenvalues of H in the smaller interval $[\beta + (\min \mu_r(\beta))^{-1}, \alpha + (\max \mu_r(\alpha))^{-1}]$, and that the numbers $\alpha + \dfrac{1}{\mu_r(\alpha)}$ and $\beta + \dfrac{1}{\mu_r(\beta)}$ provide j^+ pairs of upper and lower bounds for those eigenvalues.

From the results of section 3, it is clear that the interval $(-\beta, -\alpha)$ could be used in place of (α, β) and results parallel to those of this section would be obtained.

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(Paper 68B4–129)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 68B, No. 4, October–December 1964

The Greatest Crossnorm

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(September 8, 1964)

Let $\mathfrak{H}$ be a complex Hilbert space. If T is a completely continuous operator on $\mathfrak{H}$ then $(T^*T)^{1/2}$ is also completely continuous and nonnegative. If $\lambda_1, \lambda_2, \ldots$ represent all the nonzero eigenvalues of $(T^*T)^{1/2}$—each eigenvalue repeated in the sequence the number of times equal to its multiplicity—we may form the sum $\Sigma_i \lambda_i$ which we denote by $\tau(T)$. By definition, the *trace-class* (τc) consists of all those operators T for which $\tau(T)$ is finite. (τc) forms a linear space and $\tau(T)$ defines there a norm. The resulting normed linear space turns out to be complete, and the operators of finite rank form a dense set in (τc).

It is of significance to observe that for operators T of finite rank, $\tau(T)$ may be also expressed via concepts meaningful in a perfectly general Banach space. This observation permits then to carry over to perfectly general Banach spaces the concept of a trace-class of operators: One considers the linear space of all the operators T of finite rank on the given Banach space. There one defines $\tau(T)$ via the concepts meaningful in general Banach spaces. The customary metric completion of the so resulting normed linear space furnishes then the desired trace-class of operators.

1. Introduction

Let $\mathfrak{H}$ be a complex Hilbert space. If T is a completely continuous operator on $\mathfrak{H}$, then $(T^*T)^{1/2}$ is not only completely continuous but also nonnegative (hence Hermitean). If $\lambda_1, \lambda_2, \ldots$ represent all the nonzero eigenvalues of $(T^*T)^{1/2}$—each eigenvalue repeated in the sequence the number of times equal to its multiplicity—we may form the sum $\Sigma_i \lambda_i$ which—to indicate its dependence on the operator T—will be also denoted by $\tau(T)$. By definition, the *trace-class* (τc) consists of all those operators T for which $\tau(T)$ is finite. It is not a simple argument to prove that (τc) forms a linear space and that $\tau(T)$ defines there a norm. Incidentally, the resulting normed linear space turns out to be complete, that is, forms a Banach space. It is also true that the operators of finite rank form a dense set in (τc).

We remark that for an operator T, the above definition of $\tau(T)$ involves notions which are meaningful only in linear spaces with an inner product. It is of interest—and in fact of significance—to observe that for operators T of finite rank, $\tau(T)$ may be also expressed via concepts meaningful in a perfectly general Banach space. This means, for operators T on $\mathfrak{H}$ of finite rank, we have two versions for $\tau(T)$. While one immediately carries over to arbitrary Banach spaces, the other does not yield to a straightforward generalization. This observation permits one to carry over to perfectly general Banach spaces the concept of a trace-class of operators. To define the last, one simply proceeds as follows: One considers the linear space of all the operators T of finite rank on the given Banach space. There one defines $\tau(T)$ via the concepts meaningful in general Banach spaces. The customary metric completion of the resulting normed linear space furnishes then the desired trace-class of operators.

It remains thus to sketch how, for operators T of finite rank, $\tau(T)$ may be expressed via concepts meaningful in any Banach space. The argument follows: If $f_1, \ldots, f_n$ and $g_1, \ldots, g_n$ are elements in $\mathfrak{H}$, then

$$Tg = \sum_{i=1}^{n} (g, g_i) f_i$$

represents an operator T of finite rank which we shall also denote symbolically by $\sum_{i=1}^{n} f_i \otimes \overline{g_i}$. The converse is also true, that is, every operator T of finite rank admits many such representations of the form $\sum_{j=1}^{m} \varphi_j \otimes \overline{\chi_j}$; the number of terms m will vary of course with the representation of T. It can be shown that

$$\tau(T) = \inf \sum_{j=1}^{m} \|\varphi_j\| \, \|\chi_j\|$$

where the above infimum extends over the set of all sums corresponding to all possible representations of the operator T of finite rank.

The details of all that was said above form the main goal of this exposition.

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2. The Greatest Crossnorm

The last formula expresses $\tau(T)$ in a language meaningful for any Banach space. This suggests *the desirability of investigating the above infimum for general normed linear spaces* (not necessarily inner product spaces.) The details follow:

Let $\mathcal{F}$ and $\mathcal{G}$ stand for any two normed linear spaces and $\mathcal{F}^*$, $\mathcal{G}^*$ represent their conjugate spaces, that is, the corresponding spaces of additive and bounded, that is, continuous, linear functionals on $\mathcal{F}$ and $\mathcal{G}$ respectively.

For a fixed pair of elements $G_0 \epsilon \mathcal{G}^*$ and $f_0 \epsilon \mathcal{F}$, the expression

$$Tg = G_0(g) f_0$$

defines an operator of rank 1 from $\mathcal{G}$ into $\mathcal{F}$. More generally, if $G_1, \ldots, G_n$ are in $\mathcal{G}^*$ and $f_1, \ldots, f_n$ are in $\mathcal{F}$, then

$$Tg = \sum_{i=1}^{n} G_i(g) f_i$$

represents an operator from $\mathcal{G}$ into $\mathcal{F}$ of rank at most n. The last operator we shall also denote by $\sum_{i=1}^{n} f_i \otimes G_i$; one calls then $\sum_{i=1}^{n} f_i \otimes G_i$ a representation of the operator T. It is not difficult to see that conversely, every operator T from $\mathcal{G}$ into $\mathcal{F}$ of finite rank has many such representations. With each representation $\sum_{i=1}^{n} f_i \otimes G_i$ of a given operator T of finite rank, one associates the number $\sum_{i=1}^{n} \|f_i\| \, \|G_i\|$ and then defines

$$\gamma(T) = \inf \sum_{i=1}^{n} \|f_i\| \, \|G_i\|$$

where the infimum extends over the set of numbers corresponding to all possible representations of T. We prove below that the so defined $\gamma(T)$ is a norm on the linear space of all operators from $\mathcal{G}$ into $\mathcal{F}$ of finite rank. The metric completion of the above normed linear space is then defined as the trace-class of operators from $\mathcal{G}$ into $\mathcal{F}$.

As was already pointed out in the Introduction, one of our objectives is to show, that for the special case when both $\mathcal{F}$ and $\mathcal{G}$ represent a Hilbert space $\mathfrak{H}$, then $\gamma(T) = \tau(T)$ for every operator T on $\mathfrak{H}$ of finite rank.

Similarly, if $f_1, \ldots, f_n$ are in $\mathcal{F}$ and $g_1, \ldots, g_n$ are in $\mathcal{G}$, the expression $\sum_{i=1}^{n} f_i \otimes g_i$ represents an operator T of finite rank from $\mathcal{G}^*$ into $\mathcal{F}$ whose defining equation is given by $T(G) = \sum_{i=1}^{n} G(g_i) f_i$. Moreover, every operator T of finite rank from $\mathcal{G}^*$ into $\mathcal{F}$ has many such representations.

At this stage one should ask the following question: Assume that $f_1, \ldots, f_n$ are in $\mathcal{F}$ and $g_1, \ldots, g_n$ are in $\mathcal{G}$. Assume also that $f'_1, \ldots, f'_m$ are in $\mathcal{F}$ and $g'_1, \ldots, g'_m$ are in $\mathcal{G}$. When do the expressions $\sum_{i=1}^{n} f_i \otimes g_i$ and $\sum_{j=1}^{m} f'_j \otimes g'_j$ represent the same operator of finite rank from $\mathcal{G}^*$ into $\mathcal{F}$. To answer this question observe (writing $f_1 \otimes g_1 + \ldots + f_n \otimes g_n$ instead of $\sum_{i=1}^{n} f_i \otimes g_i$) that

$$f_1 \otimes g_1 + f_2 \otimes g_2 + \ldots + f_n \otimes g_n = f_{1'} \otimes g_{1'} + f_{2'} \otimes g_{2'} + \ldots + f_{n'} \otimes g_{n'} \quad (1)$$

where $1', 2', \ldots, n'$ is any permutation of the $1, 2, \ldots, n$.

$$f_1 \otimes (g_1 + \bar{g}_1) + f_2 \otimes g_2 + \ldots + f_n \otimes g_n = f_1 \otimes g_1 + f_1 \otimes \bar{g}_1 + f_2 \otimes g_2 + \ldots + f_n \otimes g_n. \quad (2a)$$

$$(f_1 + \bar{f}_1) \otimes g_1 + f_2 \otimes g_2 + \ldots + f_n \otimes g_n = f_1 \otimes g_1 + \bar{f}_1 \otimes g_1 + f_2 \otimes g_2 + \ldots + f_n \otimes g_n. \quad (2b)$$

$$(a_1 f_1) \otimes g_1 + (a_2 f_2) \otimes g_2 + \ldots + (a_n f_n) \otimes g_n = f_1 \otimes (a_1 g_1) + f_2 \otimes (a_2 g_2) + \ldots + f_n \otimes (a_n g_n) \quad (3)$$

where $a_1, a_2, \ldots, a_n$ are arbitrary scalars.

It is not difficult to see that two expressions $\sum_{i=1}^{n} f_i \otimes g_i$ and $\sum_{j=1}^{m} f'_j \otimes g'_j$ define the same operator T of finite rank if and only if one can be derived from the other by a finite number of successive applications of the above relations 1, 2a, 2b, 3.

The problem is to furnish some "enlightening" information concerning $\gamma(T) = \inf \sum_{i=1}^{n} \|f_i\| \, \|g_i\|$ where the infimum is extended over the set of sums corresponding to all possible representations $\sum_{i=1}^{n} f_i \otimes g_i$ of the given operator T of finite rank. In other words, we are interested in some characterizations of the above infimum. Perhaps in particular Banach spaces, it is possible to express $\gamma(T)$ *directly in terms of* T just as it was done in the case of completely continuous operators T on a Hilbert space. In the last, $\gamma(T) = \tau(T) = \sum_i \lambda_i$, where the λ_i represent all the nonzero eigenvalues of $(T^*T)^{1/2}$; each eigenvalue appearing in the last sum the number of times equal to its multiplicity.

In this connection one is tempted to add an additional problem: Suppose that $\mathcal{F}_1$ and $\mathcal{G}_1$ are subspaces of the normed linear spaces $\mathcal{F}$ and $\mathcal{G}$. If $f_1, \ldots, f_n$ are in $\mathcal{F}_1$ and $g_1, \ldots, g_n$ are in $\mathcal{G}_1$, then $\sum_{i=1}^{n} f_i \otimes g_i$ may be considered as an operator T_1 from $\mathcal{G}_1^*$ into $\mathcal{F}_1$, as well as an operator T from $\mathcal{G}^*$ into $\mathcal{F}$. Since all the representations of T_1 are among the representations of

T, it is clear that $\gamma(T) \leq \gamma(T_1)$. When are they equal? The preceding discussion and the equality $\gamma(T)=\pi(T)$ which we promise to prove later, imply that this is always the case when both $\mathscr{F}$ and $\mathscr{G}$ are Hilbert spaces.

EXAMPLE Let $\mathscr{S}$ stand for the linear space of all continuous functions $f(s)$ on $0 \leq s \leq 1$. There,

$$\|f\| = \max_{0 \leq s \leq 1} |f(s)|$$

defines a norm. Moreover, the resulting normed linear space is complete.

If $f(s)$ and $g(s)$ are both in $\mathscr{S}$, then the "product" $f(s)g(t)$ is defined and continuous on the square $0 \leq s, t \leq 1$. A function $K(s, t)$ defined on $0 \leq s, t \leq 1$ will be termed "degenerate" if it can be represented as a finite sum of products, that is, if it admits a representation of the form

$$K(s, t) = \sum_{i=1}^{n} f_i(s) g_i(t)$$

with $f_1(s), \ldots, f_n(s)$ and $g_1(s), \ldots, g_n(s)$ in $\mathscr{S}$.

It is not difficult to see that not every continuous *function* $K(s, t)$ is degenerate. It is also clear that every degenerate $K(s, t)$ admits an infinite number of representations as a finite sum of products; the number of terms in each sum will vary with the particular representation.

For each representation $\sum_{i=1}^{n} f_i(s)g_i(t)$ of a degenerate $H(s,t)$ form the number

$$\sum_{i=1}^{n} \|f_i\| \, \|g_i\| = \sum_{i=1}^{n} \max_{0 \leq s \leq 1} |f_i(s)| \cdot \max_{0 \leq s \leq 1} |g_i(s)|$$

and then consider the infimum over the set of numbers so obtained corresponding to all possible representations of the degenerate $H(s, t)$.

We are interested in some characterizations of the above infimum. In particular, we wonder whether the above infimum can be expressed *directly* in terms of a given (degenerate) $H(s, t)$.

THEOREM 1. Let $\mathscr{F}$ and $\mathscr{G}$ represent two normed linear spaces and $\mathfrak{R}$ stand for the linear space of all operators from $\mathscr{G}^*$ into $\mathscr{F}$ of finite rank. Then, the above defined function $\gamma(T)$ represents a norm on $\mathfrak{R}$. Also, $\gamma(T)$ has the "cross property," that is, $\gamma(T)$ coincides with the bound $\|T\|$ for all operators T of rank ≤ 1. The last condition characterizes $\gamma(T)$ completely in the following sense: $\gamma(T)$ is the greatest norm on $\mathfrak{R}$ having the cross property.

PROOF: Let $T \epsilon \mathfrak{R}$ and $G \epsilon \mathscr{G}^*$. Then for any representation $\sum_{i=1}^{n} f_i \otimes g_i$ of T we have

$$\|T(G)\| = \|\sum_{i=1}^{n} G(g_i) f_i\| \leq \|G\| \sum_{i=1}^{n} \|f_i\| \, \|g_i\|.$$

Thus,

$$\|T(G)\| \leq \|G\| \gamma(T).$$

The last inequality implies

$$\|T\| \leq \gamma(T)$$

for all operators T in $\mathfrak{R}$.

(i). If $T=0$, then obviously $\gamma(T)=0$. If $T \neq 0$, then $0 < \|T\| \leq \gamma(T)$, and thus $\gamma(T) > 0$.

(ii). It is also clear that for any scalar a we have $\gamma(aT) = |a| \gamma(T)$.

(iii). To prove that $\gamma(T_1 + T_2) \leq \gamma(T_1) + \gamma(T_2)$ for any two operators T_1 and T_2 in $\mathfrak{R}$, we argue as follows: Let $\epsilon > 0$ be given. Choose a representation $\sum_{i=1}^{n} f_i \otimes g_i$ of T_1, such that

$$\sum_{i=1}^{n} \|f_i\| \, \|g_i\| \leq \gamma(T_1) + \frac{\epsilon}{2}.$$

Similarly, we can find a representation $\sum_{j=1}^{m} f_j' \otimes g_j'$ of T_2 such that

$$\sum_{j=1}^{m} \|f_j'\| \, \|g_j'\| \leq \gamma(T_2) + \frac{\epsilon}{2}.$$

But, then $\sum_{i=1}^{n} f_i \otimes g_i + \sum_{j=1}^{m} f_j' \otimes g_j'$ is a representation for $T_1 + T_2$, and therefore

$$\gamma(T_1 + T_2) \leq \sum_{i=1}^{n} \|f_i\| \, \|g_i\| + \sum_{j=1}^{m} \|f_j'\| \, \|g_j'\| \leq \gamma(T_1) + \gamma(T_2) + \epsilon.$$

(iv). Assume now that T is of rank ≤ 1. Then T admits a representation in the form $T = f \otimes g$, and thus

$$\gamma(T) \leq \|f\| \, \|g\| = \|T\|.$$

We already know that $\|T\| \leq \gamma(T)$ holds. Thus $\gamma(T) = \|T\|$.

Finally, suppose that for a norm α we have $\alpha(f \otimes g) = \|f\| \, \|g\|$. Let $T \epsilon \mathfrak{R}$. For every representation $\sum_{i=1}^{n} f_i \otimes g_i$ of T we have

$$\alpha(T) = \alpha\left(\sum_{i=1}^{n} f_i \otimes g_i\right) \leq \sum_{i=1}^{n} \alpha(f_i \otimes g_i) = \sum_{i=1}^{n} \|f_i\| \, \|g_i\|.$$

Thus, $\alpha(T) \leq \gamma(T)$.

3. Some Preliminaries on Hilbert Space

The setting for our discussion is a fixed complex linear space with a complex inner product (f, g). An inner product generates a norm $\|f\| = (f, f)^{1/2}$. Of course, every norm $\|f\|$ generates a metric; the distance of two vectors f and g being given by $\|f-g\|$. We shall assume thus that our space is a Hilbert space $\mathfrak{H}$, that is, a linear space with an inner product for which the resulting metric space is complete.

In an inner product space, the following identities may be readily verified to hold for any pair of vectors f and g:

$$\|f+g\|^2 + \|f-g\|^2 = 2\|f\|^2 + 2\|g\|^2,$$

$$4(f, g) = \|f+g\|^2 - \|f-g\|^2 + i\|f+ig\|^2 - i\|f-ig\|^2.$$

The first is known as the parallelogram law. The second is known as the polarization identity.

The parallelogram law suggests that the norm on a Hilbert space is of a special kind. Obviously, not every norm on a linear space satisfies this law, and thus could not be obtained from an inner product. An early result of P. Jordan and J. von Neumann states that a Banach space (normed linear space for which the resulting metric space is complete) is a Hilbert space, that is, has a norm derivable from an inner product, if and only if the norm satisfies the parallelogram law.

A *basis* $\{\varphi_j\}$ in $\mathfrak{H}$ is by definition a maximal orthonormal family of vectors; the index set J of subscripts j is not necessarily countable. It is a consequence of Zorn's lemma (which is equivalent to Zermelo's axiom of choice) that in every Hilbert space there are bases. The cardinal number of elements in any two bases of the given space is always the same and defines the dimension of the space. Any orthonormal family of vectors in $\mathfrak{H}$ can be made part of a basis.

We mention in passing that every finite-dimensional normed linear space generates a necessarily complete metric space. Moreover, any two norms on the same finite-dimensional linear space generate equivalent topologies. More precisely: Any two normed linear spaces of the same finite dimension (and over the same scalar field) are necessarily linearly homeomorphic.

Also the following result due to Klee points out a striking difference between a finite and an infinite dimensional Hilbert space: Every infinite-dimensional Hilbert space is homeomorphic to the surface of its unit sphere, that is to the set of all f's such that $\|f\| = 1$.

To include in our discussion nonseparable spaces, that is, spaces whose bases are uncountable, we adhere to the following convention: For a family $\{\alpha_j\}$ of nonnegative numbers (where j varies over some possibly uncountable set of indices), we shall write $\sum_j \alpha_j = \alpha$ if $\alpha_j \neq 0$ for at most a countable number of indices j, and the sum formed from all the nonzero α_j, converges to α. In all other cases, we shall write $\sum_j \alpha_j = +\infty$.

Bessel's inequality

$$\sum_{i=1}^{k} |(f, \chi_i)|^2 \leq \|f\|^2$$

valid for any finite orthonormal family of vectors $\{\chi_1, \ldots, \chi_k\}$, implies that if $\{\varphi_j\}$ is a basis, then for any $f \epsilon \mathfrak{H}$, we have $(f, \varphi_j) \neq 0$ for at most a countable number of subscripts j.

The following conditions on an orthonormal family of vectors $\{\varphi_j\}$ are equivalent:

1. $\{\varphi_j\}$ is a basis in $\mathfrak{H}$.
2. $(f, \varphi_j) = 0$ for all j, implies $f = 0$.
3. For every $f \epsilon \mathfrak{H}$ we have the Fourier expansion

$$f = \sum_j (f, \varphi_j)\varphi_j.$$

4. For every pair f, g in $\mathfrak{H}$ we have Parseval's identity:

$$(f, g) = \sum_j (f, \varphi_j)(\varphi_j, g).$$

5. For every $f \epsilon \mathfrak{H}$ we have

$$\|f\|^2 = \sum_j |(f, \varphi_j)|^2.$$

We shall consider exclusively linear transformations defined on all of $\mathfrak{H}$ and having their range included in $\mathfrak{H}$. For a linear transformation A,

$$\sup_{\|f\| \leq 1} \|Af\| = \sup_{\substack{\|f\| \leq 1 \\ \|g\| \leq 1}} |(Af, g)|$$

defines its bound and is denoted by $\|A\|$. We say that A is bounded if $\|A\| < +\infty$. Boundedness is equivalent to continuity. Every linear transformation of finite rank (i.e., whose range is finite dimensional), and in particular every linear transformation on a finite dimensional space, is necessarily bounded. A bounded linear transformation will be termed an *operator*. The identity operator will be denoted by I. An operator A is invertible if there is an operator B such that $AB = BA = I$. The set of complex numbers λ for which $A - \lambda I$ is not invertible defines the spectrum of A; the last is always a closed subset of the disk $|z| \leq \|A\|$ and includes, of course, all the characteristic values of A, and perhaps other complex numbers.

If A is an operator, then there exists a unique operator A^* called the adjoint of A, such that

$$(Af, g) = (f, A^*g)$$

for all pairs of vectors f, g in $\mathfrak{H}$. We have $\|A\| = \|A^*\|$ and $\|A^*A\| = \|A\|^2$. The condition $A = A^*$ defines a Hermitean operator. If A is Hermitean, then its

spectrum is a subset of the real axis. The operator A is positive—in symbols $A \geq 0$—if $(Af,f) \geq 0$ for all f in $\mathfrak{H}$. Since $\mathfrak{H}$ is assumed to be a complex space, every positive operator A is necessarily Hermitean. An operator A is normal if $A^*A = AA^*$; we reserve the letter U for unitary operators, i.e., such that $U^*U = UU^* = I$.

For every positive operator A there is one and only one positive operator B such that $A = B^2$; we write $B = A^{1/2}$. In particular, for every operator A, the operator $(A^*A)^{1/2}$ is well defined; we find it more convenient to write $[A]$ instead of $(A^*A)^{1/2}$. Clearly, $[A] = [A^*]$ if and only if A is normal. If A is of finite rank (that is, has a finite dimensional range) then both A^*A and AA^* and therefore also $[A]$ and $[A^*]$ are of finite rank. We have $\|[A]\| = \|A\|$.

The polar decomposition of operators will play a central part in our later discussion. To state it, define an operator W to be partially isometric if W is isometric on a (closed) subspace $\mathfrak{M}$ of $\mathfrak{H}$ and equal to 0 on its orthogonal complement; $\mathfrak{M}$ is the initial set of W, while the range of W is its final set.

The polar decomposition. Let A be an operator. There exists a partially isometric operator W whose initial set is the closure of the range of $[A]$ and whose final set is the closure of the range of A, satisfying the following relations:

(i) $A = W[A]$,
(ii) $[A] = W^*A$,
(iii) $A^* = W^*[A^*]$,
(iv) $[A^*] = W[A]W^*$.

The above decomposition is unique in the following sense: If $A = W_1B_1$ where $B_1 \geq 0$ and W_1 is partially isometric having as its initial set the closure of the range of B_1, then $B_1 = [A]$ and $W_1 = W$.

In the case A is of finite rank, we may assume that W is unitary (not necessarily unique, however).

Our exposition will deal almost exclusively with completely continuous operators. Recall that a sequence $\{f_n\}$ of elements in $\mathfrak{H}$ is said to be weakly convergent in f, in symbols $f_n \rightharpoonup f$, if $(f_n,g) \to (f,g)$ for all $g \epsilon \mathfrak{H}$; as usual $f_n \to f$ will symbolize strong convergence, that is, $\|f_n - f_n\| \to 0$.

An operator A is termed completely continuous if for every bounded sequence of vectors $f_1, f_2, f_3, \ldots$ the transformed sequence $Af_1, Af_2, Af_3, \ldots$ contains a subsequence convergent (in the strong sense) to some element of the space. Equivalently, an operator A is completely continuous if it transforms every weakly convergent sequence of elements into a strongly convergent sequence, that is, $f_n \rightharpoonup f$ implies $Af_n \to Af$.

It is an immediate consequence of the polar decomposition, that one of the operators A, A^*, $[A]$, $[A^*]$ is completely continuous if and only if the same is true for the remaining three.

Definition: If φ and χ are two elements of $\mathfrak{H}$ let $\varphi \otimes \overline{\chi}$ represent the operator whose defining equation is given by

$$(\varphi \otimes \overline{\chi})f = (f, \chi)\varphi$$

for all f in $\mathfrak{H}$.

Clearly, the transformation $\varphi \otimes \overline{\chi}$ defined above, is an operator; its bound $\|\varphi \otimes \overline{\chi}\| = \|\varphi\| \|\chi\|$. The range of $\varphi \otimes \overline{\chi}$ is of dimension 1 or 0.

Remark. Observe the slight change of notation from the one introduced in 2. Riesz' representation theorem states that a linear functional $F_0(\varphi)$ defined for all $\varphi \epsilon \mathfrak{H}$, is bounded if and only if there is a unique $\chi_0 \epsilon \mathfrak{H}$ such that

$$F_0(\varphi) = (\varphi, \chi_0) \text{ for all } \varphi \epsilon \mathfrak{H}.$$

The correspondence $\chi_0 \leftrightarrow F_0$ is not an isomorphism but a conjugate-isomorphism between $\mathfrak{H}$ and $\mathfrak{H}^*$, because $\chi_0 \leftrightarrow F_0$ implies $\lambda\chi_0 \leftrightarrow \overline{\lambda}F_0$ for any complex λ. We shall thus write $\varphi \otimes \overline{\chi}$, to remind us that the χ plays the part of a bounded linear functional on $\mathfrak{H}$.

The following relations are immediate consequences of the definition of $\varphi \otimes \overline{\chi}$:

(i) $(\varphi \otimes \overline{\chi})^* = \chi \otimes \overline{\varphi}$.
(ii) $(\lambda\varphi) \otimes \overline{\chi} = \lambda(\varphi \otimes \overline{\chi})$.
(ii′) $\varphi \otimes \overline{(\lambda\chi)} = \overline{\lambda}(\varphi \otimes \overline{\chi})$.
(iii) $(\varphi_1 + \varphi_2) \otimes \overline{\chi} = \varphi_1 \otimes \overline{\chi} + \varphi_2 \otimes \overline{\chi}$.
(iii′) $\varphi \otimes \overline{(\chi_1 + \chi_2)} = \varphi \otimes \overline{\chi}_1 + \varphi \otimes \overline{\chi}_2$.
(iv) $(\varphi_1 \otimes \overline{\chi}_1)(\varphi_2 \otimes \overline{\chi}_2) = (\varphi_2, \chi_1)\varphi_1 \otimes \overline{\chi}_2$.
(v) $A(\varphi \otimes \overline{\chi}) = (A\varphi) \otimes \overline{\chi}$.
(vi) $(\varphi \otimes \overline{\chi})A = \varphi \otimes \overline{(A^*\chi)}$.

The meaning of the symbol $\sum_{i=1}^{n} \lambda_i \varphi_i \otimes \overline{\chi}_i$ is then clear; it represents an operator of rank at most n (i.e., whose range is at most n-dimensional).

In general, analogous infinite sums have no meaning. However, the following theorem will be useful for all our purposes:

THEOREM 2. Let $\{\varphi_i\}$ and $\{\chi_i\}$ stand for any two orthonormal familes of vectors and $\{\mu_i\}$ a *bounded* family of complex numbers indexed by the same set of subscripts. Then,

$$Tf = \sum_i \mu_i (f, \chi_i)\varphi_i$$

is meaningful for every f in $\mathfrak{H}$ and represents an operator T which we shall also denote by

$$\sum_i \mu_i \varphi_i \otimes \overline{\chi}_i.$$

The bound of T is given by

$$\|T\| = \sup_i |\mu_i|.$$

PROOF: We have:

$$\sum_i |\mu_i (f, \chi_i)|^2 \leq$$

$$\sup_i |\mu_i|^2 \sum_i |(f, \chi_i)|^2 \leq \|f\|^2 \sup_i |\mu_i|^2.$$

Thus Tf is meaningful and

$$\|Tf\|^2 \leq \|f\|^2 \sup_i |\mu_i|^2.$$

This of course means that $\|T\| \leq \sup_i |\mu_i|$. On the other hand, we have $\|T\chi_i\| = |\mu_i|$. And therefore $\|T\| \geq \sup_i |\mu_i|$. Thus, $\|T\| = \sup_i |\mu_i|$.

The fundamental theorem of algebra implies that the characteristic equation of a complex matrix possesses at least one (in general, complex) root. It follows that an operator on a finite-dimensional (complex) space has at least one proper value. In general if $\lambda_1, \lambda_2, \ldots, \lambda_k$ are different proper values of A and $\varphi_1 \varphi_2, \ldots, \varphi_k$ corresponding proper vectors (that is, $A\varphi_i = \lambda_i\varphi_i$) then $\varphi_1, \varphi_2, \ldots, \varphi_k$ are linearly independent. In the case an inner product space is infinite dimensional, it is always possible to construct completely continuous operators which do not have a single proper value. It may be added that thus far it is not known whether every operator T on a Hilbert space $\mathfrak{H}$ possesses a proper invariant subspace. We mean hereby, a subspace $\mathfrak{M}$ such that $0 \neq \mathfrak{M} \neq \mathfrak{H}$ and $T(\mathfrak{M}) \subset \mathfrak{M}$.

Added in proof: The September 1964 issue of the Bulletin of the American Mathematical Society, carries a research communication by Louis de Branges and James Rovnyak to the effect that every operator (linear and bounded) in a Hilbert space admits proper invariant subspaces.

The story is however quite different when one deals with Hermitean operators. The spectral theorem in its simplest version states that a *Hermitean operator* A *on a finite-dimensional unitary space admits a basis* (*orthonormal*) *in that space, made up of proper vectors of* A. We mean hereby, that there is an orthonormal basis $\varphi_1, \ldots \varphi_n$ for which $A\varphi_i = \lambda_i\varphi_i$ for $1 \leq i \leq n$, and thus

$$A = \sum_{i=1}^{n} \lambda_i \varphi_i \otimes \overline{\varphi}_i.$$

The corresponding proper values $\lambda_1, \ldots, \lambda_n$ are necessarily real.

Conversely, every sum of the above form with $\varphi_1, \ldots, \varphi_n$ orthonormal and $\lambda_1, \ldots, \lambda_n$ real, represents a Hermitean operator.

The infinite-dimensional extension of the above result which follows is also well known:

THEOREM 3. Every Hermitean completely continuous operator A on a Hilbert space admits in that space an orthonormal basis of characteristic vectors. The corresponding nonzero (necessarily real) proper values are each of finite multiplicity and may be arranged either in a finite or denumerably infinite sequence $\lambda_1, \lambda_2, \ldots$ (each nonzero characteristic value being repeated in the sequence the number of times equal to its miltiplicity) such that $\lambda_i \to 0$. If $\varphi_1, \varphi_2, \ldots$ is a corresponding orthonormal sequence of proper vectors (that is, $A\varphi_i = \lambda_i\varphi_i$ for $i = 1, 2, \ldots$), then

$$A = \sum_i \lambda_i \varphi_i \otimes \overline{\varphi}_i$$

Conversely, every sum of the above form, that is, with $\{\varphi_i\}$ orthonormal, λ_i real and $\lambda_i \to 0$, represents a completely continuous Hermitean operator.

The above yields a representation characterizing the completely continuous Hermitean operators. To obtain an analogous representation valid for all completely continuous operators, one makes use of the polar decomposition for operators.

THEOREM 4. An operator A is completely continuous if and only if it admits a *polar representation*.

$$A = \sum_i \lambda_i \varphi_i \otimes \overline{\chi}_i$$

where both $\{\varphi_i\}$ and $\{\chi_i\}$ are orthonormal sequences and the λ_i's are positive. The sum has either a finite or denumerably infinite number of terms. In the last case, we have also $\lambda_i \to 0$. The above representation is unique in the sense that the λ_i's are necessarily all the positive proper values (each represented in the sequence $\{\lambda_i\}$ the number of times equal to its multiplicity) of $[A]$.

PROOF: Since A is completely continuous, the same is true for $[A]$. Thus,

$$[A] = \sum_i \lambda_i \chi_i \otimes \overline{\chi}_i.$$

Now, if $A = W[A]$ is its polar decomposition, then W is isometric on the closed linear manifold determined by $\{\chi_i\}$. Thus, $\{W\chi_i\}$ is also an orthonormal family. Put $W\chi_i = \varphi_i$. Then

$$A = W[A] = W\left(\sum_i \lambda_i \chi_i \otimes \overline{\chi}_i\right)$$

$$= \sum_i \lambda_i (W\chi_i) \otimes \overline{\chi}_i = \sum_i \lambda_i \varphi_i \otimes \chi_i.$$

4. The Schmidt-Class and the Trace-Class of Operators

LEMMA. Let A be a given operator and $\{\varphi_i\}$, $\{\chi_j\}$ be any two bases. Then

$$\sum_i \|A\varphi_i\|^2$$

$$\sum_i \sum_j |(A\varphi_i, \chi_j)|^2$$

$$\sum_j \|A^*\chi_j\|^2$$

represent the same (finite or infinite) value; we denote the last by $|A|^2$.

PROOF. For a fixed i, the "Pythagorean theorem" implies

$$\|A\varphi_i\|^2 = \sum_j |(A\varphi_i, \chi_j)|^2$$

and thus,

$$\sum_i \|A\varphi_i\|^2 = \sum_i \sum_j |(A\varphi_i, \chi_j)|^2.$$

Replacing in the last, A by A^*, $\{\varphi_i\}$ by $\{\chi_j\}$, and $\{\chi_j\}$

by $\{\varphi_i\}$ one gets

$$\sum_j \|A^*\chi_j\|^2 = \sum_i \sum_j |(A^*\chi_j, \varphi_i)|^2$$

$$= \sum_i \sum_j |(\chi_j, A\varphi_i)|^2 = \sum_i \sum_j |(A\varphi_i, \chi_j)|^2.$$

Thus, the values of the above three sums are the same. Observe finally that, $A^{**} = A$. This concludes the proof.

Definition. For a given operator A, let $|A|^2$ stand for the common value of the three "sums" determined above.

LEMMA. For any operator A, we have $\|A\| \leq |A|$.

PROOF. It is sufficient to prove that $\|A\varphi\| \leq |A|$ for every vector φ such that $\|\varphi\| = 1$. This is easy: Choose a basis $\{\varphi_i\}$ with φ as one of its elements. Then

$$\|A\varphi\|^2 \leq \sum_i \|A\varphi_i\|^2 = |A|^2.$$

LEMMA. For any two operators A and B we have

$$|A+B| \leq |A| + |B|.$$

PROOF. It is sufficient to consider the case in which both $|A| < +\infty$ and $|B| < +\infty$. Choose a fixed basis $\{\varphi_i\}$. Then

$$|A+B| = \left(\sum_i \|(A+B)\varphi_i\|^2\right)^{1/2}$$

$$\leq \left(\sum_i (\|A\varphi_i\| + \|B\varphi_i\|)^2\right)^{1/2}$$

$$\leq \left(\sum_i \|A\varphi_i\|^2\right)^{1/2} + \left(\sum_i \|B\varphi_i\|^2\right)^{1/2} = |A| + |B|.$$

THEOREM 5. Let $\mathfrak{B}$ stand for the set of all operators A for which $|A| < +\infty$. With the obvious definitions of addition and scalar multiplication, $\mathfrak{B}$ is a complex linear space. There $|A|$ represents a norm. The norm also satisfies the parallelogram law,

$$|A+B|^2 + |A-B|^2 = 2|A|^2 + 2|B|^2.$$

PROOF. That $|A|$ is a norm on $\mathfrak{B}$ follows from the preceding propositions. The last equality is also true, since if $\{\varphi_j\}$ is a fixed basis, then for every j

$$\|A\varphi_j + B\varphi_j\|^2 + \|A\varphi_j - B\varphi_j\|^2 = 2\|A\varphi_j\|^2 + 2\|B\varphi_j\|^2.$$

THEOREM 6. Let A and B be two operators in $\mathfrak{B}$ and $\{\varphi_j\}$ a given basis. Then

$$(A, B) = \sum_j (A\varphi_j, B\varphi_j)$$

is a well-defined complex number, independent of the chosen basis. Also, (A, B) defines an inner product on $\mathfrak{B}$ and thus

$$|A| = (A, A)^{1/2}$$

is the norm which it generates.

PROOF. For each j we have

$$4(A\varphi_j, B\varphi_j) = \|A\varphi_j + B\varphi_j\|^2$$

$$- \|A\varphi_j - B\varphi_j\|^2 + i\|A\varphi_j + iB\varphi_j\|^2 - i\|A\varphi_j - iB\varphi_j\|^2$$

and thus,

$$4(A, B) = |A+B|^2 - |A-B|^2 + i|A+iB|^2 - i|A-iB|^2.$$

Remark. Incidentally, the inner product space $\mathfrak{B}$ is also complete (hence a Banach space); it contains the operators of finite rank as a dense subset. Considering however, $\mathfrak{B}$ only as a *linear* set of operators on $\mathfrak{H}$, and defining the bound $\|A\|$ of an operator as a new norm on $\mathfrak{B}$, then the resulting normed linear space is *not* complete, (provided $\mathfrak{H}$ is infinite-dimensional).

Remark. Incidentally, $|A|$ also satisfies the following conditions:

(i) $|A| = |A^*|$.

(ii) For any operator B, we have

$$|AB| \leq |A|\,\|B\| \leq |A|\,|B|.$$

As a consequence of (ii), $\mathfrak{B}$ is also an algebra. In fact, $\mathfrak{B}$ is an ideal in the algebra of all operators.

Definition: An operator A in $\mathfrak{B}$ is commonly referred to as one which belongs to the *E. Schmidt-class* and $|A|$ is said to define its Hilbert-Schmidt norm.

Remark. That the Hilbert-Schmidt norm of an operator is always not smaller than its bound was proven above. Also, it can be readily verified that the Hilbert-Schmidt norm is a crossnorm; that is, $|A| = \|A\|$ wherever A is an operator of rank ≤ 1.

At this point, the following comment is in order: Let L_2 stand for the Hilbert space of all complex-valued Lebesgue measurable functions $f(x)$ defined on the interval $0 \leq x \leq 1$ for which $|f(x)|^2$ is integrable; two functions being considered identical if and only if they differ on a set of measure zero. There, the linear operations are the usual ones in function spaces; the inner product is represented by

$$(f, g) = \int f(x)\overline{g(x)}dx.$$

Similarly, let $\mathscr{L}_2$ represent the Hilbert space of complex-valued measurable functions $K(x,y)$ defined on $0 \leq x,\ y \leq 1$ for which $|K(x,y)|^2$ is integrable; the inner product being given by

$$(H, K) = \iint H(x, y)\,\overline{K(x, y)}\,dx\,dy.$$

One observes that if $K_1(x,y)$ and $K_2(x,y)$ are both in $\mathscr{L}_2$, then the function

$$H(x, y) = \int K_1(x, z)K_2(z, y)\,dz$$

is also in $\mathscr{L}_2$ and

$$\iint |H(x, y)|^2 dx\,dy$$

$$\leq \iint |K_1(x, y)|^2 dx\,dy \cdot \iint |K_2(x, y)|^2 dx\,dy.$$

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Thus, if $H(x,y)$ is defined as the "product" of $K_1(x,y)$ and $K_2(x,y)$, the space $\mathcal{L}_2$ turns out to be an algebra.

Let $K(x,y)$ be a fixed element in $\mathcal{L}_2$. For $f(x)$ in L_2,

$$\int K(x, y) f(y)\, dy$$

is then defined for almost all x in $0 \leq x \leq 1$ and represents a function $g(x)$, again in L_2. It turns out that the equation

$$g(x) = \int K(x, y) f(y)\, dy$$

defines an operator K on L_2 which belongs to the Schmidt-class (of operators on L_2) and

$$|K| = (\int\int |K(x, y)|^2 dx\, dy)^{1/2}.$$

Moreover, every operator on L_2 in the Schmidt-class is obtained in such a manner. This one-to-one correspondence between $\mathcal{L}_2$ and the Schmidt-class of operators on L_2 preserves addition, scalar-multiplication, products, and the norm. This means we have the following:

THEOREM 7. The Schmidt-class of operators on L_2, and the Hilbert space $\mathcal{L}_2$, are congruent not only as Banach spaces but also as Banach algebras.

THEOREM 8. Every operator A in the Schmidt-class is necessarily completely continuous.

PROOF. Let $f_n \rightharpoonup f$. We prove the following: Given an $\epsilon > 0$, there is a natural number n_0 such that for all $n > n_0$ one has $\|Af_n - Af\| < \epsilon$.

Clearly for some constant c we have $\|f_n\| \leq c$ for all n and thus also $\|f\| \leq c$. Choose a basis $\{\varphi_j\}$. Since A is in the Schmidt-class, we can find a finite set J of indices j such that

$$\Sigma_{j \in J} \|A\varphi_j\|^2 < \frac{\epsilon^2}{16\, c^2}.$$

Clearly,

$$f_n - f = \Sigma_j (f_n - f, \varphi_j)\varphi_j$$

and therefore,

$$Af_n - Af = \Sigma_j (f_n - f, \varphi_j) A\varphi_j.$$

Thus, for every natural n,

$$\|Af_n - Af\|^2 = \|\Sigma_{j \in J}(f_n - f, \varphi_j)A\varphi_j + \Sigma_{j \notin J}(f_n - f, \varphi_j)A\varphi_j\|^2$$

$$\leq 2\|\Sigma_{j \in J}(f_n - f, \varphi_j)A\varphi_j\|^2 + 2\|\Sigma_{j \notin J}(f_n - f, \varphi_j)A\varphi_j\|^2.$$

The second term on the right of the last inequality is

$$\leq 2\|f_n - f\|^2 \Sigma_{j \in J}\|A\varphi_j\|^2 \leq 2(2c)^2 \frac{\epsilon^2}{16c^2} = \frac{\epsilon^2}{2}.$$

On the other hand $f_n \rightharpoonup f$ implies $\lim_n (f_n - f, \varphi_j) = 0$ for all j. Thus, the sum

$$2\|\Sigma_{j \in J}(f_n - f, \varphi_j)A\varphi_j\|^2$$

having a finite number of terms can be made $< \frac{\epsilon^2}{2}$ for large enough n, say for all $n > n_0$. Therefore for all $n > n_0$, we have

$$\|Af_n - Af\|^2 < \epsilon^2.$$

The theorem which follows characterizes the completely continuous operators in the Schmidt-class.

THEOREM 9. A completely continuous operator $A = \Sigma_i \lambda_i \varphi_i \otimes \overline{\chi_i}$ belongs to the Schmidt-class if and only if $\Sigma_i \lambda_i^2 < +\infty$, that is, the series formed from the non-zero proper values of A^*A converges. In the last case we also have

$$|A| = (\Sigma_i \lambda_i^2)^{1/2}.$$

PROOF. We extend $\{\chi_i\}$ to a basis by adding $\{\omega_j\}$. Of course

$$\|A\chi_i\| = \|\lambda_i \varphi_i\| = \lambda_i \text{ and } \|A\omega_j\| = 0.$$

Hence,

$$|A|^2 = \Sigma_i \|A\chi_i\|^2 + \Sigma_j \|A\omega_j\|^2 = \Sigma_i \lambda_i^2.$$

COROLLARY. The operators of finite rank form a dense set in the Schmidt-class.

PROOF. Let $A = \Sigma_i \lambda_i \varphi_i \otimes \overline{\chi_i}$ with $\Sigma_i \lambda_i^2 < +\infty$. Let $A_n = \sum_{i=1}^{n} \lambda_i \varphi_i \otimes \overline{\chi_i}$.

Then,

$$\lim_n |A - A_n| = \lim_n (\Sigma_{i>n} \lambda_i^2)^{1/2} = 0.$$

LEMMA. Let A be a given operator and $\{\varphi_i\}$ a basis. Then

$$\Sigma_i ([A]\varphi_i, \varphi_i)$$

is independent of the chosen basis.

PROOF. Since $[A] \geq 0$, there is a unique operator $B \geq 0$ such that $[A] = B^2$. Now,

$$([A]\varphi_i, \varphi_i) = (B^2\varphi_i, \varphi_i) = (B\varphi_i, B\varphi_i) = \|B\varphi_i\|^2$$

and $\Sigma_i \|B\varphi_i\|^2$ is of course independent of the chosen basis $\{\varphi_i\}$.

Definition. The operators A for which the sum in the preceding Lemma is finite, form the trace-class (τc).

THEOREM 10. Let (τc) denote the class of all operators A for which

$$\tau(A) = \Sigma_j ([A]\varphi_j, \varphi_j) < +\infty$$

for a fixed basis $\{\varphi_j\}$. With the obvious definition of addition and scalar multiplication, (τc) is a linear space. The last will be normed if the above sum represents the norm of an operator A. Moreover, the resulting normed linear space is complete, hence a Banach space: it contains the operators of finite rank as a dense subset. The operators in the trace-class necessarily belong to the Schmidt-class, and thus are

completely continuous. Moreover (τc) is a (two-sided) ideal in the algebra of all operators and a Banach algebra under its own norm.[2]

THEOREM 11. Every operator in the trace-class is necessarily in the Schmidt-class. Every operator in the Schmidt-class is completely continuous.

Let A be a completely continuous operator and $\Sigma_i \lambda_i \varphi_i \otimes \overline{\chi}_i$ its polar form. Then A is in the Schmidt-class if and only if $\Sigma_i \lambda_i^2 < +\infty$; we have $|A| = (\Sigma_i \lambda_i^2)^{1/2}$ The operator A is in the trace-class if and only if $\Sigma_i \lambda_i < +\infty$; we have $\tau(A) = \Sigma_i \lambda_i$.

THEOREM 12. For an operator T of finite rank

$$\tau(T) = \gamma(T) = \inf \sum_{j=1}^{m} \|f_j\| \, \|g_j\|$$

where the infimum is taken over the set of all numbers corresponding to all possible representations $\sum_{j=1}^{m} f_j \otimes \overline{g}_j$ of T.

PROOF. Since $\tau(T)$ is a crossnorm, for any representation $\sum_{j=1}^{m} f_j \otimes \overline{g}_j$ of T we have $\tau(T) \leq \sum_{j=1}^{m} \tau(f_j \otimes \overline{g}_j) = \sum_{j=1}^{m} \|f_j\| \, \|g_j\|$. Thus, $\tau(T) \leq \gamma(T)$. However, if $\sum_{i=1}^{n} \lambda_i \varphi_i \otimes \overline{\chi}_i$ is a polar representation of T, then

$$T^*T = \left(\sum_{i=1}^{n} \lambda_i \chi_i \otimes \overline{\varphi}_i \right) \left(\sum_{i=1}^{n} \lambda \varphi_i \otimes \overline{\chi}_i \right)$$

$$= \sum_{i=1}^{n} \lambda_i^2 \chi_i \otimes \overline{\chi}_i$$

and $[T] = \sum_{i=1}^{n} \lambda_i \chi_i \otimes \overline{\chi}_i$. Now, $[T]\varphi = 0$ whenever φ is orthogonal to $\chi_1, \ldots, \chi_n$. Thus,

$$\tau(T) = \sum_{i=1}^{n} ([T]\chi_i, \chi_i)$$

$$= \sum_{i=1}^{n} (\lambda_i \chi_i, \chi_i) = \sum_{i=1}^{n} \lambda_i$$

$$= \sum_{i=1}^{n} \|\lambda_i \varphi_i\| \, \|\chi_i\| \geq \gamma(T).$$

This concludes the proof.

(Paper 68B4–130)

[2] For the complete details of the proof of Theorem 10, the reader is advised to consult this author's monograph "Norm Ideals of Compietely Continuous Operators" Ergebnisse der Mathematik (Springer-Verlag, Berlin, 1960).

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 68B, No. 4, October–December 1964

Publications of the National Bureau of Standards*

Selected Abstracts

Relaxation modes of trapped crystal point defects: the three-neighbor shells model in NaCl. A. D. Franklin, A. Shorb, and J. B. Wachtman, Jr., *J. Res. NBS* **69A** (*Phys. and Chem.*), *No. 5, (Sept.-Oct. 1964), 70 cents.*

The results of a relaxation mode analysis are presented for two cases of trapped-defect relaxation in the NaCl structure, in which both defects occupy the same type of site (e.g., impurity divalent ion and trapped vacancy), or in which they occupy the two different types of sites (vacancy pair.) The relaxation analysis is presented in the form of a set of basis vectors in occupation-probability space and a set of secular equations. Solutions to the equations provide the relaxation rates and also the coefficients in the linear combinations of the basis vectors which constitutes the relaxation modes.

Calculations of the relaxation rates and contributions to the polarizability of the various modes for a three-shell model with jump frequencies chosen to represent the relaxation of an impurity-ion vacancy pair in NaCl(Mn) have confirmed the results of Lozovskii. Even though the third shell makes a significant and even large contribution to the process, one mode dominates and the relaxation as seen in a-c measurements would take place with essentially a single relaxation time. The d-c techniques of Dreyfus are sensitive enough to detect more than one of these relaxations at low temperatures, but the slowest of these will always be the dominant one. *Any relaxation slower than the major one must be ascribed to some other mechanism.*

Miscellaneous studies in probability and statistics, *NBS Tech. Note 238 (Apr. 24, 1964), 20 cents.*

This publication makes available some notes and tables prepared at various times by the staff of the Statistical Engineering Laboratory. Contents: (1) Distribution of the ratio of two F variates having $n-1$ and n degrees of freedom, by J. M. Cameron and Cyrus Derman. (2) Some notes on the Cauchy distribution, by Cyrus Derman. Includes variance of the sample mean for truncated Cauchy distribution; the Cauchy distribution whose cumulative distribution function deviates least from the standard normal *c.d.f.* (3) The better one out of two, by E. P. King. Variance of the observation closest to the population mean. (4) Variance of medians and pseudo-medians, by Mary G. Natrella. For sample sizes m up to 10, gives the variances (5D) of the median (m odd), pseudo-median (m even), and average of two values on either side of the median (m odd), for the normal and rectangular distributions and ($m \leq 6$) for the extreme-value distribution. (5) Probability points of order statistics in random samples of size n from a uniform distribution over (0,1), by Churchill Eisenhart and Lola S. Deming. Gives probability points (4S) of each order statistic for probabilities $\alpha = .001, .005, .01, .025, .05, .10, .20, .25, .50$, and $n = 2(1)10$.

Handbook of mathematical functions with formulas, graphs, and mathematical tables, Ed. M. Abramowitz and I. A. Stegun, *NBS Applied Math. Series 55, (June 1964), $6.50.*

This publication not only combines the material found in all former reference volumes on the subject; it additionally expands the work of past authors by increasing the number of functions covered, presenting more extensive numerical tables, and giving larger collections of mathematical properties of the tabulated functions. It also provides comparatively simple methods of obtaining values of functions outside the tabulated range.

As a result of scientific advances and, especially, the increasing use of automatic computers, a greater variety of functions and a higher accuracy of tabulation are now in demand by users of mathematical functions. The *Handbook* includes rational approximation formulas for all the functions, tailored to the modern computer and tables useful for a pre-programming survey of the access to a computer; for the researcher who does not, and who must do his own computations, they are, of course, indispensable. Subjects covered are included by the following chapter headings: Mathematical Constants; Physical Constants and Conversion Factors; Elementary Analytical Methods; Elementary Transcendental Functions-Logarithmic, Exponential, Circular, and Hyperbolic Functions; Exponential Integral and Related Functions; Gamma Function and Fresnel Integrals; Legendre Functions; Bessel Functions of Integer Order; Bessel Functions of Fractional Order; Integrals of Bessel Functions; Struve Functions and Related Functions; Confluent Hypergeometric Functions; Coulomb Wave Functions; Hypergeometric Functions; Jacobian Elliptic Functions and Theta Functions; Elliptic Integrals; Weierstrass Elliptic and Related Functions; Parabolic Cylinder Functions; Mathieu Functions; Spheroidal Wave Functions; Orthogonal Polynomials; Bernoulli and Euler Polynomials, Riemann Zeta Functions; Combinatorial Analysis; Numerical Interpolation, Differentiation, and Integration; Probability Functions; Miscellaneous Functions; Scales of Notation, and Laplace Transforms.

Computation of Hankel function, L. A. Berry, *NBS Tech. Note 216 (June 12, 1964), 20 cents.*

Methods of computing solutions to Bessel's equation, $z^2\frac{d^2y}{dz^2}+z\frac{dy}{dz}+(z^2-v^2)y=0$, for complex v and z, and for small, real v, are given in detail. The methods are most suitable for use on an electronic digital computer. With a computer which carries eight decimal digits, the methods presented for small, real v will return at least six correct significant digits for all z. When v and z are both complex, the accuracy depends on $|z|$ (since asymptotic forms are used) and the ratio v/z. Relative error curves are shown as a function of $|v/z|$ parametric in $|z|$. For v sufficiently far from z, seven correct digits are obtained, which for $v \cong z$, the relative error is of the order $10^{-2}/|z|$.

Weierstrass points of $\Gamma_0(n)$, J. Lehner and M. Newman, *Ann. Math.* **79,** *No. 2, 360–368 (Mar. 1964).*

The principal results of the paper ar that 0 is in general a Weierstrass point of $\Gamma_0(n)$ when n is divisible by 4 or by 9, and that if n is prime then $\Gamma_0(n)$ is hyperelliptic if and only if $n = 23, 29, 31, 41, 47, 71$.

A two-parameter family of hyper-Poisson distributions, G. E. Bardwell and E. L. Crow, *J. Am. Stat. Assoc.* **59,** *133–141 (Mar. 1964).*

A two-parameter generalization of the Poisson distributions, called the "Hyper-Poisson" family, is derived and discussed. It is in turn a special case of the three-parameter confluent hypergeometric series distributions. When one parameter is fixed, the hyper-Poisson distributions are also power series distributions. The distributions are classified as "sub-Poisson" or "super-Poisson" according as the variance is less than or greater than the mean. The latter category includes the truncated Poisson distributions. Certain properties of the hyper-Poisson distributions are considered, including moment, modified moment, and maximum likelihood estimators of the parameters. Estimation using moments is illustrated on Student's haemacytometer data.

Exact conditions for the preservation of a canonical distribution in Markovian relaxation processed, H. C. Andersen, I. Oppenheim, K. E. Shyler, and G. H. Weiss, *J. Math. Phys.* **5,** *No. 4, 522–536 (Apr. 1964).*

Necessary and sufficient conditions have been determined for the exact preservation of a canonical distribution characterized by a time-dependent temperature (canonical invariance) in Markovian relaxation processes governed by a master equation. These conditions, while physically realizable, are quite restrictive so that canonical invariance is the exception rather than the rule. For processes with a continuous energy variable, canonical invariance requires that the integral master equation is exactly equivalent to a Fokker-Planck equation with linear transition moments of a special form. For processes with a discrete energy variable, canonical invariance requires, in addition to a special form of the level degeneracy, equal spacing of the energy levels and transitions between nearest-neighbor levels only. Physically, these conditions imply that canonical invariance is maintained only for weak interactions of a special type between the relaxing subsystem and the reservoir. It is also shown that canonical invariance is a sufficient condition

for the exponential relaxation of the mean energy. A number of systems (hard-sphere Rayleigh gas, Brownian motion, harmonic oscillators, nuclear spins) are discussed in the framework of the above theory. Conditions for *approximate* canonical invariance valid up to a certain order in the energy are also developed and then applied to nuclear spins in a magnetic field.

Pointwise bounds in the first biharmonic boundary value problem, J. H. Bramble and L. E. Payne, *J. Math. Phys.* **42,** *No. 4, 278–286 (Dec. 1963).*

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Bounds at interior points are also given for derivatives up to order three.

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Phase fluctuation statistics. J. B. Smyth.

Current topics in the stochastic theory of radiation. F. J. Zucker.

On the intensity distribution

$$\frac{2R}{\sqrt{\alpha\beta}}\exp\left[-\frac{R^2}{2}\left(\frac{1}{\alpha}+\frac{1}{\beta}\right)\right]I_0\left(\frac{R^2}{2}\left[\frac{1}{\beta}-\frac{1}{\alpha}\right]\right)$$

and its application to signal statistics. M. Nakagami.

Statistical inference for Rayleigh distributions. M. M. Siddiqui.

A probabilistic approach to the problem of large antenna arrays. Y. T. Lo.

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Library of Congress Catalog Card Number: 62–4414

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C., 20402. Price 75 cents (single copy). Subscription price: $2.25 a year, $0.50 additional for foreign mailing.

UNITED STATES GOVERNMENT PRINTING OFFICE, WASHINGTON : 1964